9-1215

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: SABIHA QAZI Examiner # : 74141 Date: 9/22/06

Art Unit: 1616 Phone Number: 2-0622 Serial Number: 10/821,479

Location (Bldg/Room#): 4A45 (Mailbox #): 4C70 Results Format Preferred (circle): PAPER DISK

****

Rem

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: MG

Title of Invention: 2-Propylidene-19-nor-Vitamin D compds

Inventors (please provide full names): DeLuca et al

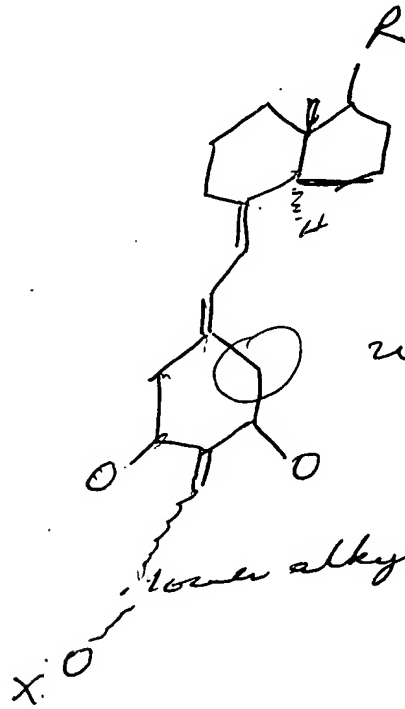
Earliest Priority Date: 4/10/2003

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only ***Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.***

Please search for 19-nor Vit D compds of cl 1 and their method of use



Broad Search

no 19 CH_2 gp (called 19-nor Vit D)

For Specific Compds See compds of cl 12-16.

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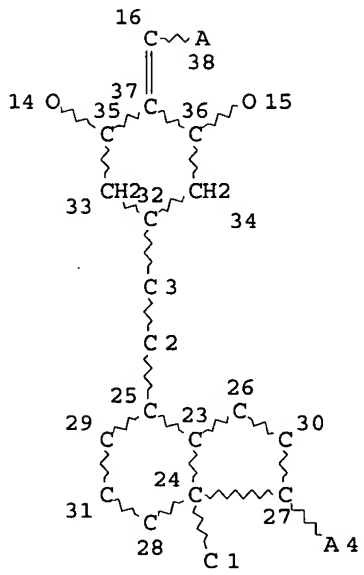

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L16 8 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND L2
L17 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L16

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L17 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:376695 HCAPLUS
DOCUMENT NUMBER: 145:83577

TITLE: New 2-Alkylidene 1α,25-Dihydroxy-19-norvitamin D3 Analogues of High Intestinal Activity: Synthesis and Biological Evaluation of 2-(3'-Alkoxypropylidene) and 2-(3'-Hydroxypropylidene) Derivatives

AUTHOR(S): Glebocka, Agnieszka; Sicinski, Rafal R.; Plum, Lori A.; Clagett-Dame, Margaret; DeLuca, Hector F.

CORPORATE SOURCE: Department of Biochemistry, University of Wisconsin-Madison, Madison, WI, 53706, USA

SOURCE: Journal of Medicinal Chemistry (2006), 49(10), 2909-2920
CODEN: JMCMAR; ISSN: 0022-2623

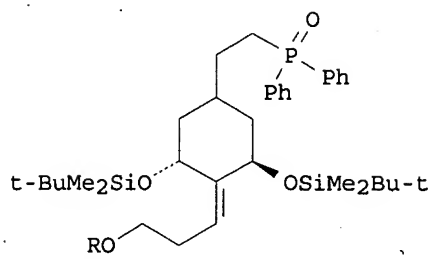
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:83577

GI



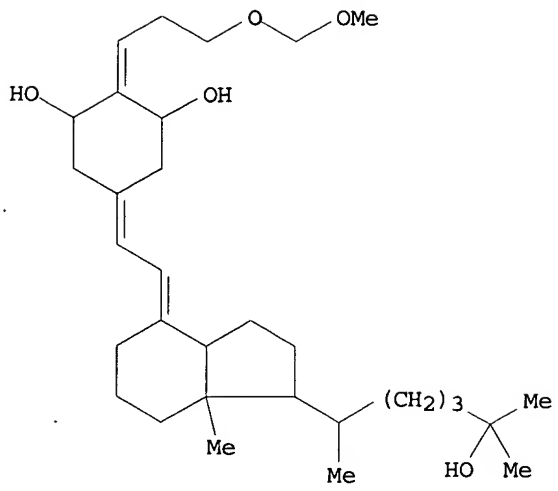
I

AB In a search for novel vitamin D compds. of potential therapeutic value, E- and Z-isomers of 1α,25-dihydroxy-2-(3'-hydroxypropylidene)-19-norvitamin D3, as well as a derivative of the former compound possessing a 3'-(methoxymethoxy)propylidene substituent at C-2, were efficiently prepared All vitamins were obtained in convergent syntheses, starting with (-)-quinic acid and the protected 25-hydroxy Grundmann ketones. Phosphine oxides I were prepared and subjected to Lythgoe type Wittig-Horner coupling with CD-ring fragments. An alternative route was also elaborated that comprised Julia coupling of sulfones with a cyclohexanone derivative The binding of all synthesized vitamins to the full-length rat recombinant vitamin D receptor (VDR) is either similar to or within one log of 1α,25(OH)2D3. The in vivo tests have revealed that the calcemic activity of all analogs in the E-series is considerably higher than that of the native hormone.

IT **766529-87-7P 781664-40-2P 781664-41-3P 781664-71-9P 781664-72-0P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. evaluation of 2-alkoxypropylidene and 2-hydroxypropylidene 1α,25-dihydroxy-19-norvitamin D3 analogs)

RN 766529-87-7 HCAPLUS

CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-[3-(methoxymethoxy)propylidene]-, (1α,3bβ,6E,7E)-(9CI) (CA INDEX NAME)



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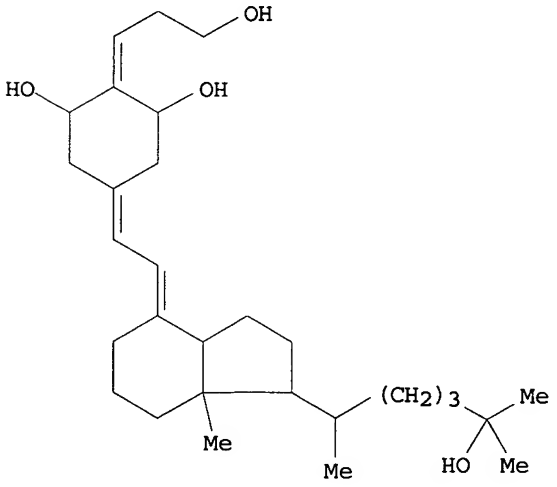
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2E,3β,7E)- (9CI) (CA INDEX NAME)



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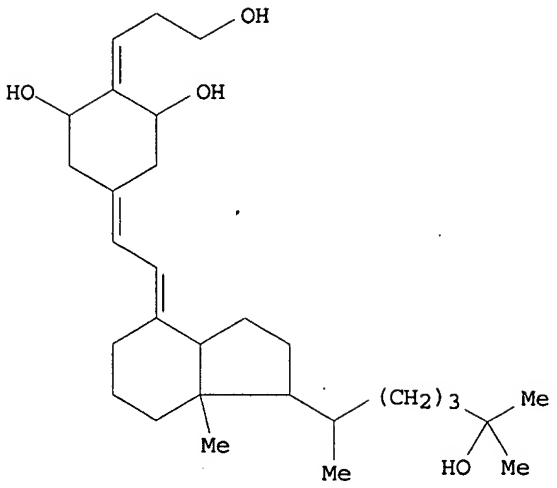
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)



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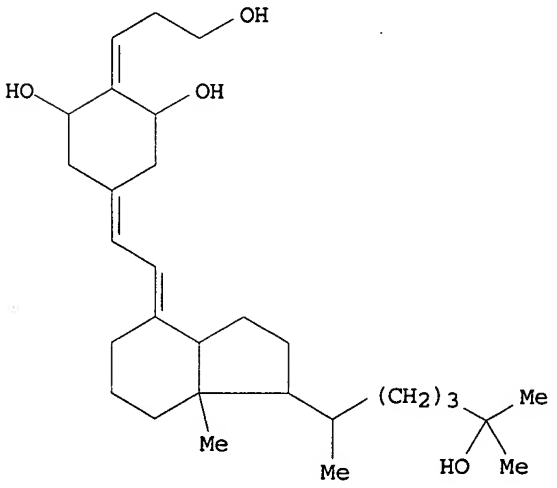

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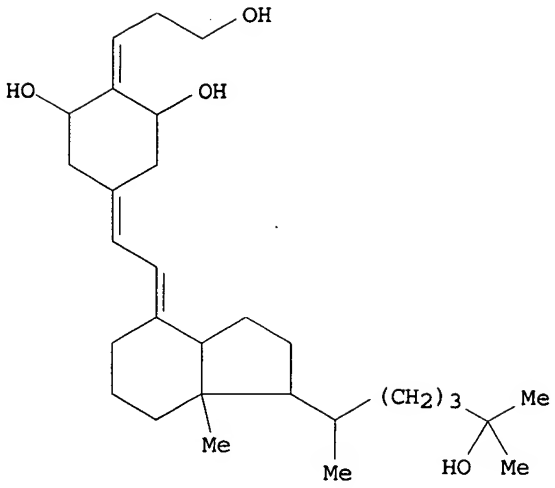
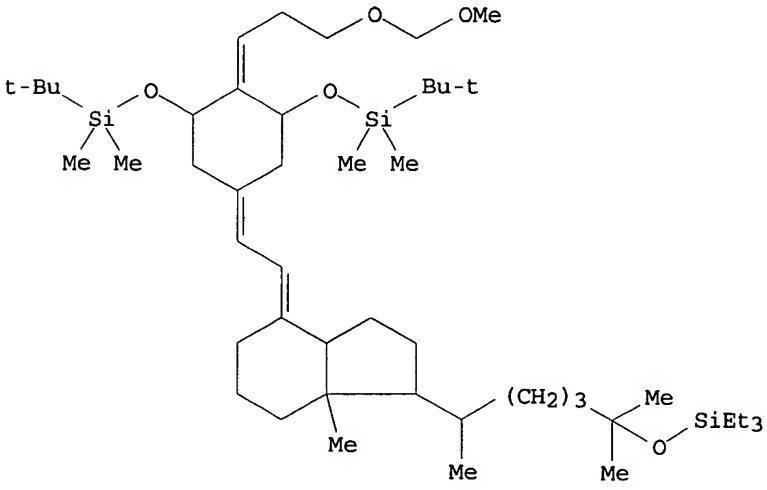
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



IT **766529-93-5P 781664-39-9P 781664-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and biol. evaluation of 2-alkoxypropylidene and 2-hydroxypropylidene 1α,25-dihydroxy-19-norvitamin D3 analogs)

RN 766529-93-5 HCAPLUS
CN Silane, [[(1α,3β,6E,7E)-2-[3-(methoxymethoxy)propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7,10(19)-triene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



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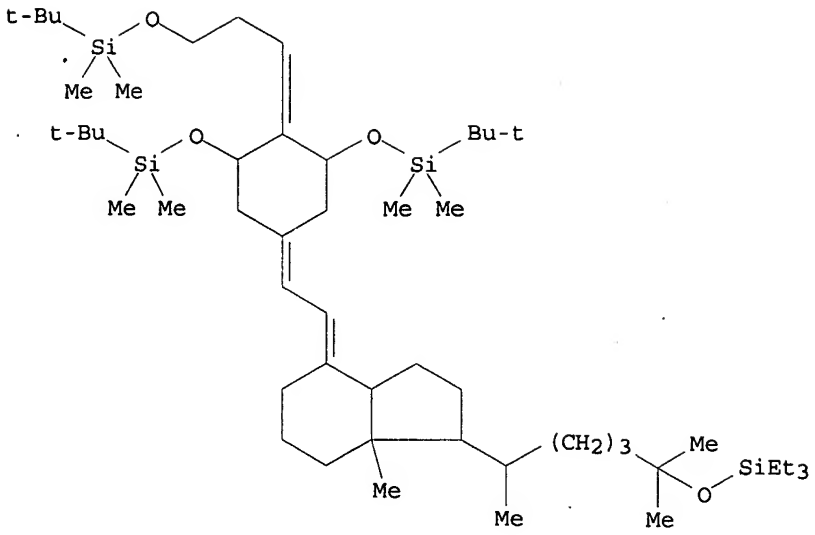
CN Silane, [[(1α,2E,3β,7E)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



RN 781664-70-8 HCAPLUS
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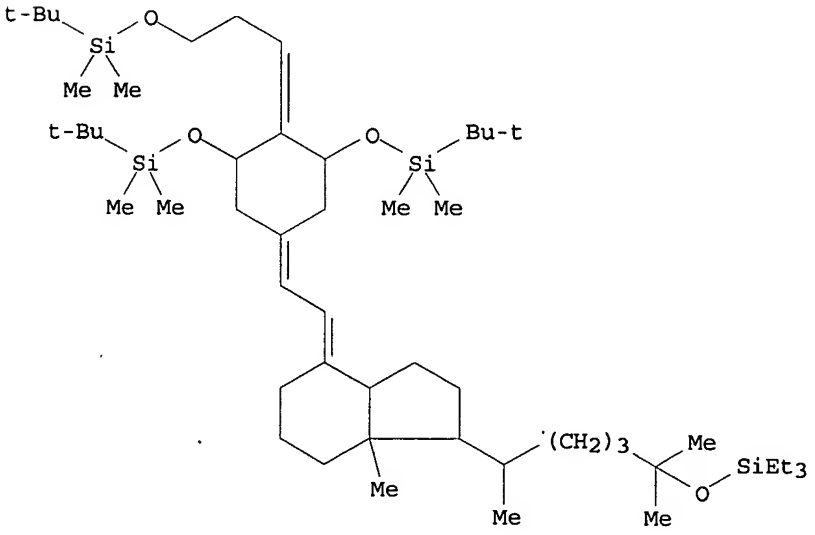

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Section cross-reference(s): 2
IT **766529-87-7P 781664-40-2P 781664-41-3P 781664-71-9P 781664-72-0P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and biol. evaluation of 2-alkoxypropylidene and 2-hydroxypropylidene 1α,25-dihydroxy-19-norvitamin D3 analogs)
IT 78365-43-2P 120379-76-2P 163217-18-3P 194227-13-9P

766529-88-8P 766529-89-9P 766529-90-2P 766529-91-3P
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780781-81-9P 780781-82-0P 780781-84-2P 781664-36-6P
781664-37-7P 781664-38-8P **781664-39-9P** 781664-42-4P
781664-70-8P 892501-31-4P 892501-32-5P 892501-33-6P
892501-34-7P 892501-35-8P 892501-36-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and biol. evaluation of 2-alkoxypropylidene and 2-hydroxypropylidene 1α,25-dihydroxy-19-norvitamin D3 analogs)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:474934 HCAPLUS
DOCUMENT NUMBER: 143:20385
TITLE: Vitamin d analogs for obesity prevention and treatment
INVENTOR(S): Deluca, Hector F.; Clagett-Dame, Margaret; Ahrens, Jamie M.; Ntambi, James M.; Thomson, Brian
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 102 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005119242	A1	20050602	US 2004-997698	2004 1124
AU 2004293092	A1	20050609	AU 2004-293092	2004 1124
CA 2544502	AA	20050609	CA 2004-2544502	2004 1124
WO 2005051396	A2	20050609	WO 2004-US39524	2004 1124
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US 7053075	B2	20060530		
EP 1689412	A2	20060816	EP 2004-812196	2004 1124

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	US 2003-524813P	P	2003 1125
	WO 2004-US39524	W	2004 1124
	WO 2004-US39625	W	2004 1124

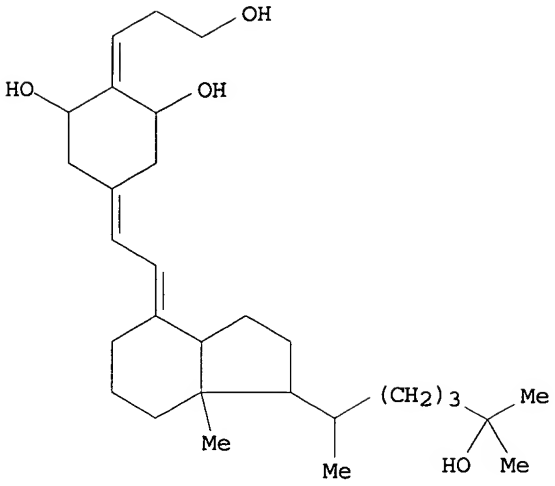
OTHER SOURCE(S): MARPAT 143:20385

AB Methods for treating and preventing obesity, inhibiting adipocyte differentiation, inhibiting increased SCD-1 gene transcription, and/or reducing body fat in a subject include administering at least one analog of 1α,25-dihydroxyvitamin D3, 1α,25-dihydroxyvitamin D2, or 19-nor vitamin D or a pharmaceutical composition that includes such an analog to a subject in need thereof are disclosed.

IT **781664-41-3P 781664-72-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(vitamin D analogs for obesity prevention and treatment)

RN 781664-41-3 HCAPLUS

CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)



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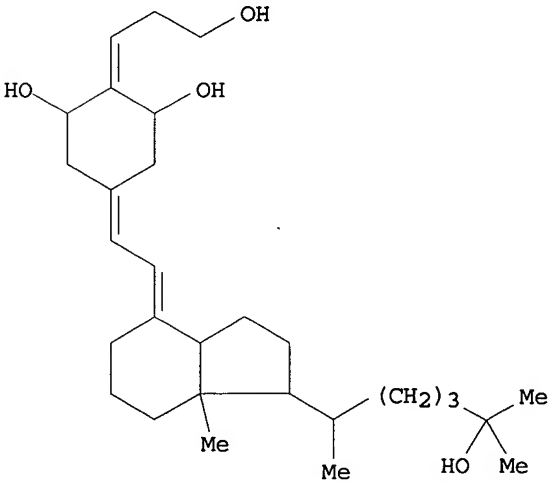
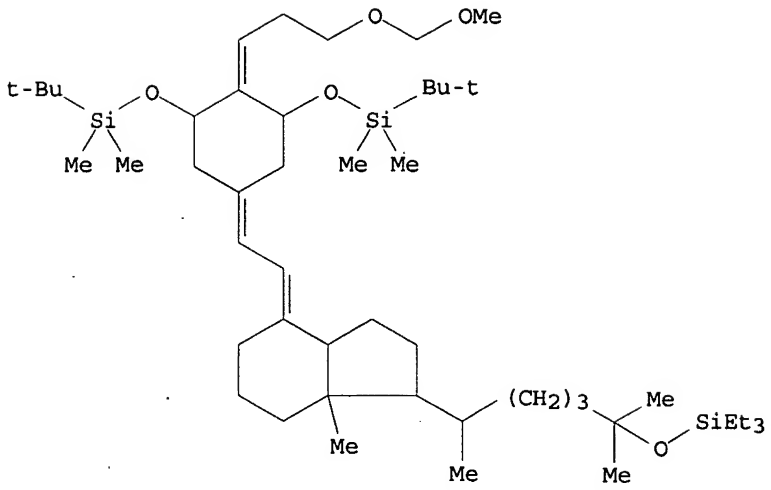
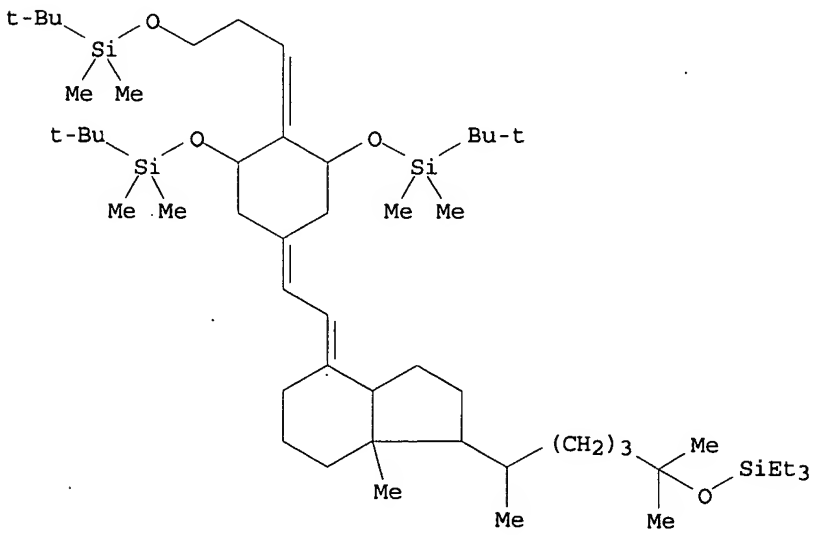
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



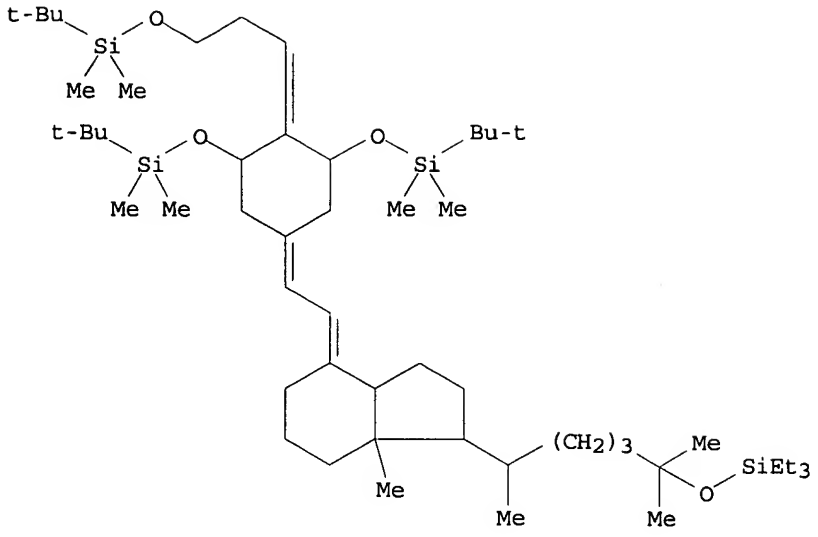
IT **766529-93-5P 781664-39-9P 781664-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vitamin D analogs for obesity prevention and treatment)
RN 766529-93-5 HCAPLUS
CN Silane, [[(1α,3β,6E,7E)-2-[3-(methoxymethoxy)propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7,10(19)-triene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



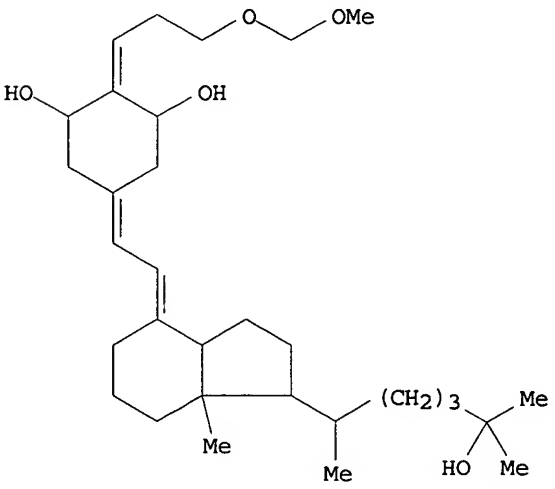
RN 781664-39-9 HCAPLUS
CN Silane, [[(1α,2E,3β,7E)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



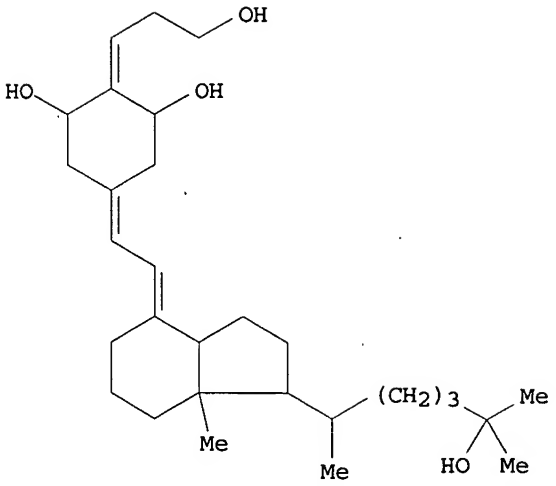
RN 781664-70-8 HCAPLUS
CN Silane, [[(1α,2E,3β,7E,20S)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



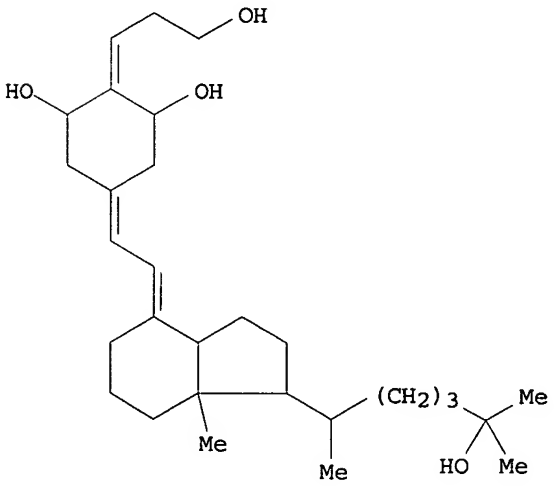
IT **766529-87-7 781664-40-2 781664-71-9**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(vitamin D analogs for obesity prevention and treatment)
RN 766529-87-7 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,
2-[3-(methoxymethoxy)propylidene]-, (1α,3bβ,6E,7E)-
(9CI) (CA INDEX NAME)



RN 781664-40-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,
2-(3-hydroxypropylidene)-, (1α,2E,3β,7E)- (9CI) (CA
INDEX NAME)



RN 781664-71-9 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)



IC ICM A61K031-59
INCL 514167000
CC 2-10 (Mammalian Hormones)
Section cross-reference(s): 1, 63
IT 213250-70-5P 524067-20-7P 524067-21-8P 524067-22-9P
736995-69-0P **781664-41-3P 781664-72-0P**
852658-44-7P 852658-46-9P 852658-48-1P 852658-50-5P
852658-51-6P 852658-52-7P 852658-54-9P 852658-70-9P
852932-06-0P 852947-04-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(vitamin D analogs for obesity prevention and treatment)
IT 64190-52-9P 66774-70-7P 66774-71-8P 66774-80-9P
78365-43-2P 100928-03-8P 104651-47-0P 120379-76-2P
145354-28-5P 163217-18-3P 171011-48-6P 185997-26-6P
186372-30-5P 189102-57-6P 194227-13-9P 197647-61-3P

213250-64-7P 214351-86-7P 235108-01-7P 303780-38-3P
618879-43-9P 766529-88-8P 766529-89-9P 766529-90-2P
766529-91-3P 766529-92-4P **766529-93-5P** 766529-94-6P
766529-95-7P 766529-96-8P 766529-97-9P 780781-79-5P
780781-80-8P 780781-81-9P 780781-82-0P 780781-83-1P
780781-84-2P 781664-36-6P 781664-37-7P 781664-38-8P
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781664-45-7P **781664-70-8P** 852658-59-4P 852658-60-7P
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852658-65-2P 852658-66-3P 852658-67-4P 852658-68-5P
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852658-90-3P 852658-91-4P 852658-92-5P 852658-93-6P
852658-94-7P 852658-95-8P 852658-96-9P 852658-97-0P
852658-98-1P 852658-99-2P 852659-00-8P 852659-01-9P
852659-02-0P 852659-03-1P 852659-04-2P 852932-04-8P
852932-07-1P 852932-08-2P 852932-09-3P 852932-10-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vitamin D analogs for obesity prevention and treatment)

IT 60133-18-8D, 1α-25-Dihydroxyvitamin D2, analog 131918-61-1
766529-87-7 781664-40-2 781664-71-9
845815-92-1 852932-01-5 852932-02-6 852932-03-7
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(vitamin D analogs for obesity prevention and treatment)

L17 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:902336 HCAPLUS
DOCUMENT NUMBER: 141:380071
TITLE: Preparation of 2-propylidene-19-norvitamin D compounds for pharmaceutical use
INVENTOR(S): Deluca, Hector F.; Sicinski, Rafal R.; Glebocka, Agnieszka; Plum, Lori A.
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

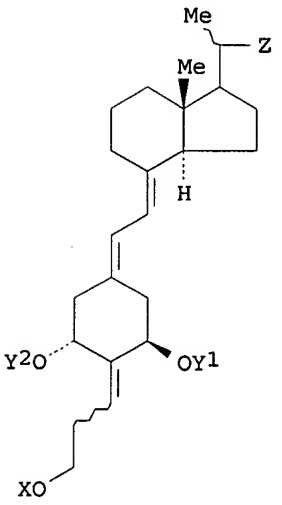
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092118	A2	20041028	WO 2004-US11059	2004 0409
WO 2004092118	A3	20050127		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004230948	A1	20041028	AU 2004-230948	2004 0409

CA 2516233	AA	20041028	CA 2004-2516233	2004 0409
US 2004229851	A1	20041118	US 2004-821479	2004 0409
EP 1613588	A2	20060111	EP 2004-749961	2004 0409
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004009194	A	20060411	BR 2004-9194	2004 0409
CN 1771226	A	20060510	CN 2004-80009620	2004 0409

PRIORITY APPLN. INFO.:	US 2003-461958P	P 2003 0410
	US 2004-821479	A 2004 0409
	WO 2004-US11059	A 2004 0409

OTHER SOURCE(S): MARPAT 141:380071

GI



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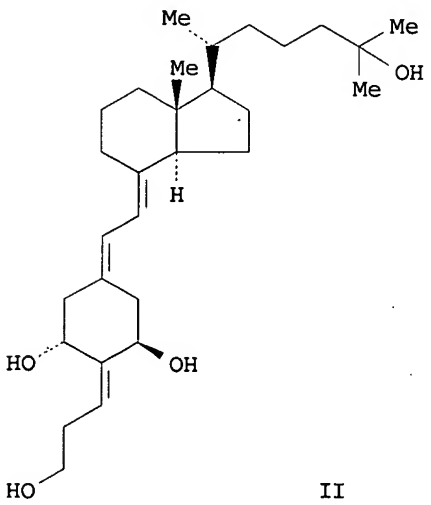


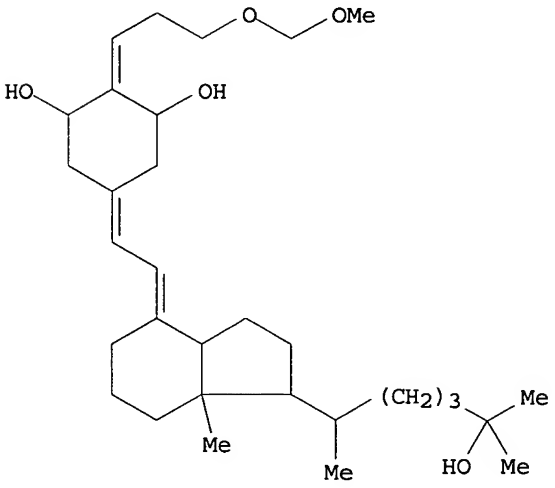
II

AB 2-Propylidene-19-norvitamin D compds. of formula I [Y1, Y2 = H, protecting group; X = H, alkyl, protecting group, hydroxyalkyl, alkoxyalkyl, aryloxyalkyl; Z = H, Me, acyl, (substituted) OH, CH2OH, etc.] are prepared for pharmaceutical use. These compds. are characterized by high bone calcium mobilization activity and high intestinal calcium transport activity. This results in novel therapeutic agents for the treatment and prophylaxis of diseases

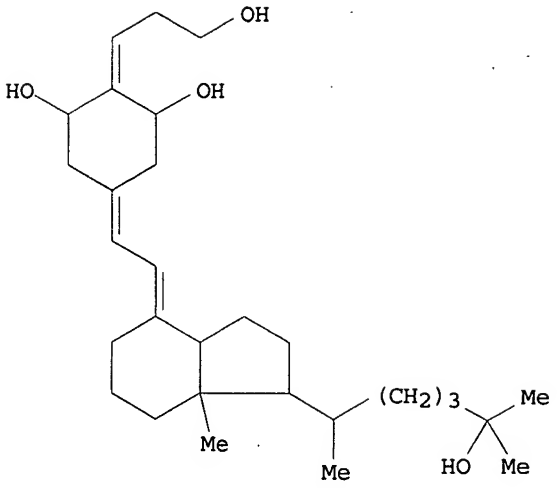
where bone formation is desired, particularly osteoporosis, as well as autoimmune diseases such as multiple sclerosis, diabetes mellitus and lupus. These compds. also exhibit pronounced activity in arresting the proliferation of undifferentiated cells and inducing their differentiation to the monocyte thus evidencing use as an anti-cancer agent and for the treatment of skin diseases such as psoriasis. These compds. also increase both breaking strength and crushing strength of bones evidencing use in conjunction with bone replacement surgery such as hip and knee replacements. Thus, II was prepared and showed significant activity in promoting the differentiation of leukemia cells.

IT **766529-87-7P 781664-40-2P 781664-41-3P 781664-71-9P 781664-72-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-propylidene-19-norvitamin D compds. as antiosteoporotics and antitumor agents)

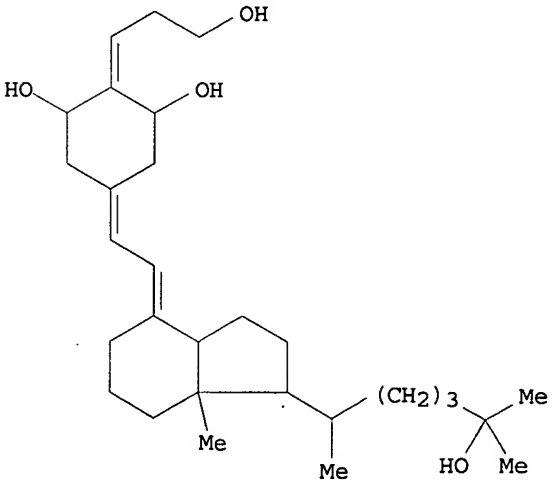
RN 766529-87-7 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-[3-(methoxymethoxy)propylidene]-, (1α,3bβ,6E,7E)- (9CI) (CA INDEX NAME)



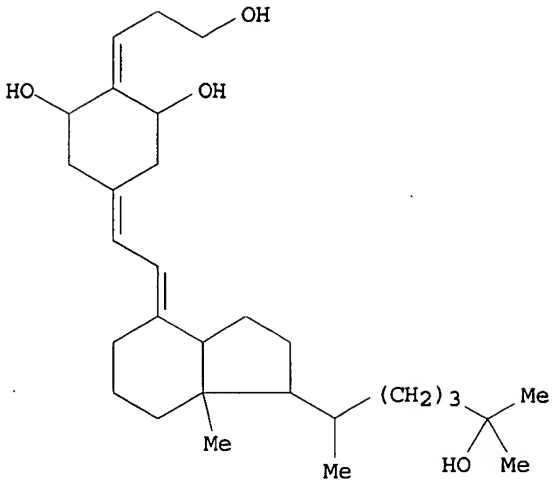
RN 781664-40-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2E,3β,7E)- (9CI) (CA INDEX NAME)



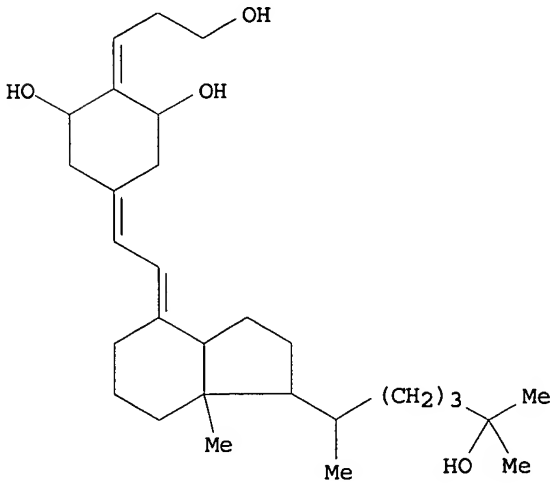
RN 781664-41-3 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)



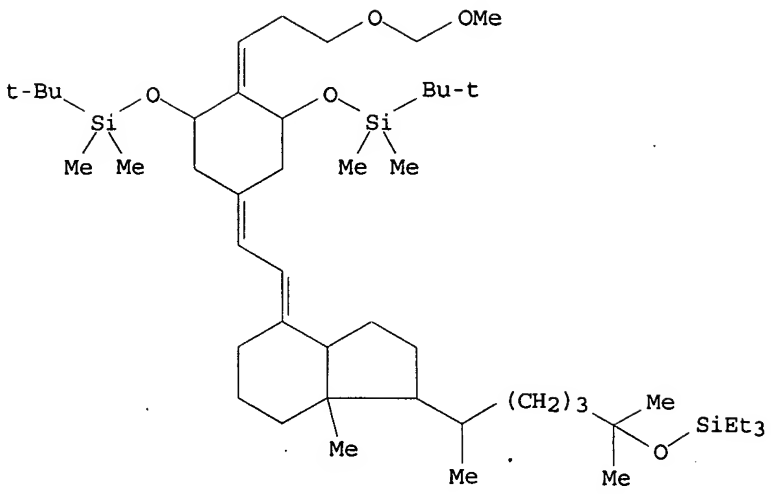
RN 781664-71-9 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)



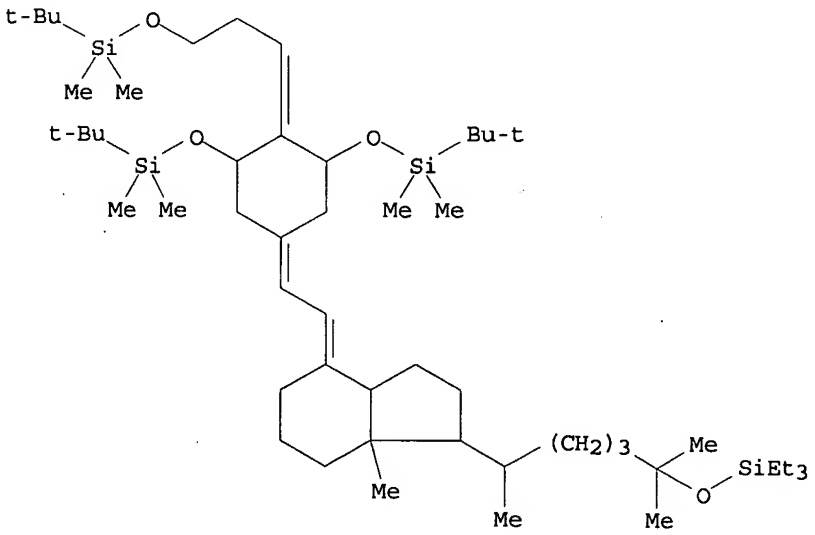
RN 781664-72-0 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(3-hydroxypropylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



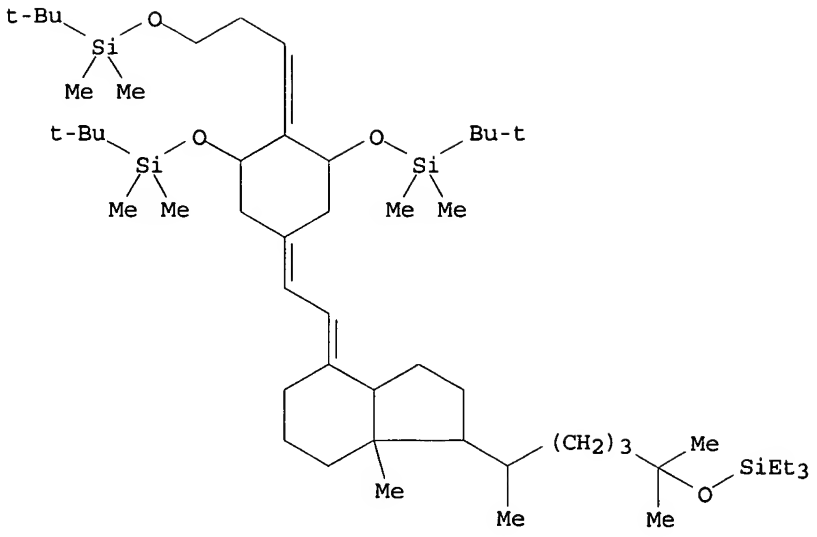
IT **766529-93-5P 781664-39-9P 781664-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-propylidene-19-norvitamin D compds. as antiosteoporotics and antitumor agents)
RN 766529-93-5 HCAPLUS
CN Silane, [[(1α,3β,6E,7E)-2-[3-(methoxymethoxy)propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7,10(19)-triene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 781664-39-9 HCAPLUS
CN Silane, [[(1α,2E,3β,7E)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



RN 781664-70-8 HCAPLUS
CN Silane, [[(1α,2E,3β,7E,20S)-2-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



IC ICM C07C401-00
CC 32-7 (Steroids)
Section cross-reference(s): 1, 63
IT **766529-87-7P 781664-40-2P 781664-41-3P**
781664-71-9P 781664-72-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-propylidene-19-norvitamin D compds. as antiosteoporotics and antitumor agents)
IT 78365-43-2P 120379-76-2P 163217-18-3P 194227-13-9P
766529-88-8P 766529-89-9P 766529-90-2P 766529-91-3P
766529-92-4P **766529-93-5P** 766529-94-6P 766529-95-7P
766529-96-8P 766529-97-9P 780781-79-5P 780781-80-8P
780781-81-9P 780781-82-0P 780781-84-2P 781664-36-6P
781664-37-7P 781664-38-8P **781664-39-9P** 781664-42-4P
781664-43-5P 781664-44-6P **781664-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-propylidene-19-norvitamin D compds. as antiosteoporotics and antitumor agents)

L17 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:522163 HCAPLUS
DOCUMENT NUMBER: 141:314479
TITLE: New derivative of 1α,25-dihydroxy-19-norvitamin D3 with 3'-alkoxypropylidene moiety at C-2: synthesis, biological activity and conformational analysis
AUTHOR(S): Glebocka, Agnieszka; Sicinski, Rafal R.; DeLuca, Hector F.
CORPORATE SOURCE: Department of Biochemistry, University of Wisconsin-Madison, Madison, WI, 53706, USA
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (2004), 89-90(1-5), 25-30
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: : Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:314479
GI

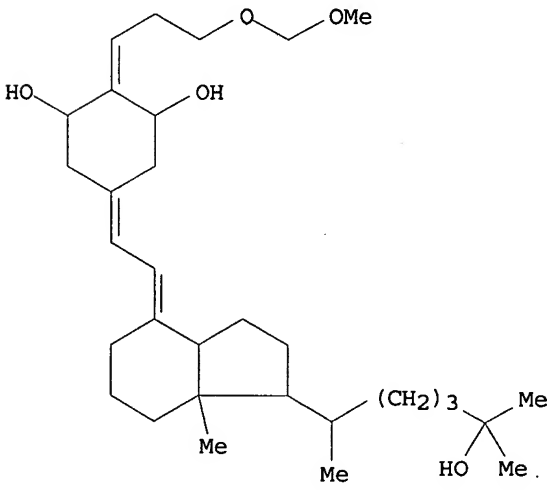
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

AB In pursuit of novel biol. active Vitamin D compds. of potential therapeutic value, 1α,25-dihydroxy-2-[3'-(methoxymethoxy)propylidene]-19-norvitaminD3 (I) was efficiently prepared in a convergent synthesis, starting with (-)-quinic acid and the protected 25-hydroxy Grundmann ketone I. The key synthetic step involved Lythgoe type Wittig-Horner coupling of II, with the phosphine oxide III (R = SiCMe3Me2). Mol. modeling was employed to establish the A-ring conformation of the synthesized Vitamin I. Also, preliminary modeling of its complex with the rVDR was performed and interactions between ligand and the binding domain analyzed. Analog I was found to be only six times less potent than 1α,25-(OH)2D3 in binding to the rat recombinant Vitamin D receptor (VDR). In comparison with hormone 1α,25-(OH)2D3, it also showed slightly lower cellular HL-60-differentiation activity. Preliminary in vivo tests indicated unusually high calcemic activity of I.

IT **766529-87-7P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of a norvitamin D3 analog with 3'-alkoxypropylidene moiety at C-2 from (-)-quinic acid; its binding to the vitamin D receptor, and conformational anal.)

RN 766529-87-7 HCAPLUS

CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-[3-(methoxymethoxy)propylidene]-, (1α,3bβ,6E,7E)-(9CI) (CA INDEX NAME)

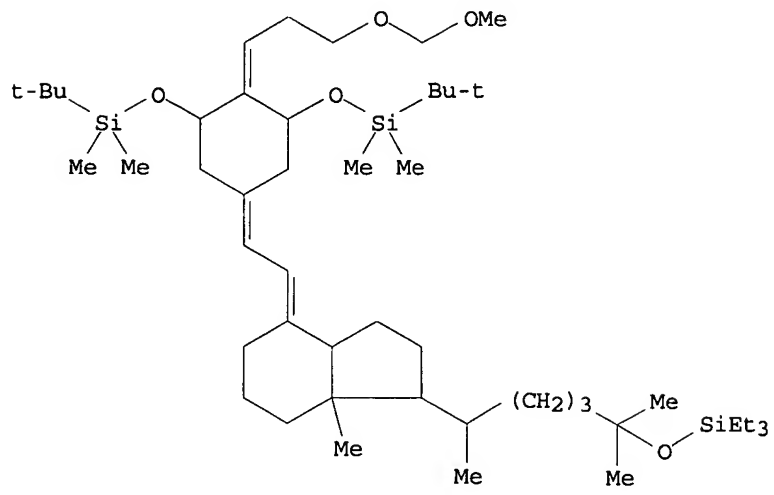


IT **766529-93-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a norvitamin D3 analog with 3'-alkoxypropylidene moiety at C-2 from (-)-quinic acid; its binding to the vitamin D receptor, and conformational anal.)

RN 766529-93-5 HCAPLUS

CN Silane, [[(1α,3β,6E,7E)-2-[3-(methoxymethoxy)propylidene]-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7,10(19)-triene-1,3-diyl]bis(oxy)]bis[(1,1-

dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



CC 32-7 (Steroids)
IT **766529-87-7P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of a norvitamin D3 analog with 3'-alkoxypropylidene moiety at C-2 from (-)-quinic acid; its binding to the vitamin D receptor, and conformational anal.)
IT 665-27-0P 163217-18-3P 766529-88-8P 766529-89-9P
766529-90-2P 766529-91-3P 766529-92-4P **766529-93-5P**
766529-94-6P 766529-95-7P 766529-96-8P 766529-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a norvitamin D3 analog with 3'-alkoxypropylidene moiety at C-2 from (-)-quinic acid; its binding to the vitamin D receptor, and conformational anal.)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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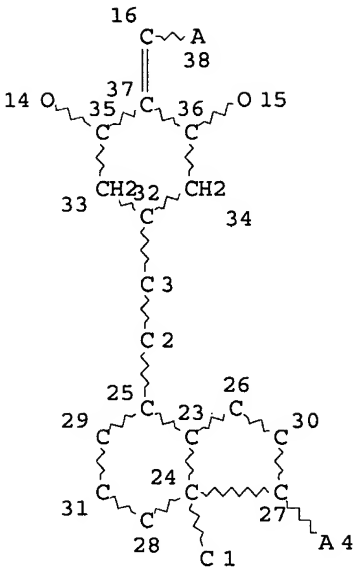

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

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L16	8	SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND L2
L17	4	SEA FILE=HCAPLUS ABB=ON PLU=ON L16
L18	10	SEA FILE=HCAPLUS ABB=ON PLU=ON L15
L19	6	SEA FILE=HCAPLUS ABB=ON PLU=ON L18 NOT L17

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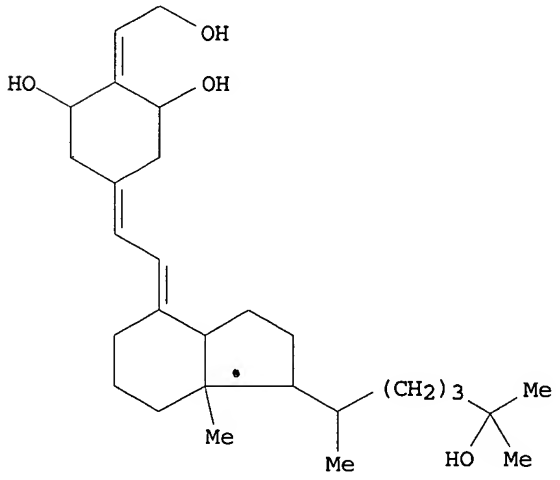
L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:505971 HCAPLUS
DOCUMENT NUMBER: 145:201953
TITLE: Analogs of 1α,25-dihydroxyvitamin D3 with high potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation: Synthesis and biological evaluation of 2-substituted 19-norvitamin D analogs
AUTHOR(S): Shimazaki, Mika; Miyamoto, Yukiko; Yamamoto, Keiko; Yamada, Sachiko; Takami, Masamichi; Shinki, Toshimasa; Udagawa, Nobuyuki; Shimizu, Masato
CORPORATE SOURCE: Institute of Biomaterials and Bioengineering Tokyo Medical and Dental University, Chiyoda-ku, Tokyo, 101-0062, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(13), 4645-4656
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In our previous papers, we found that introduction of a

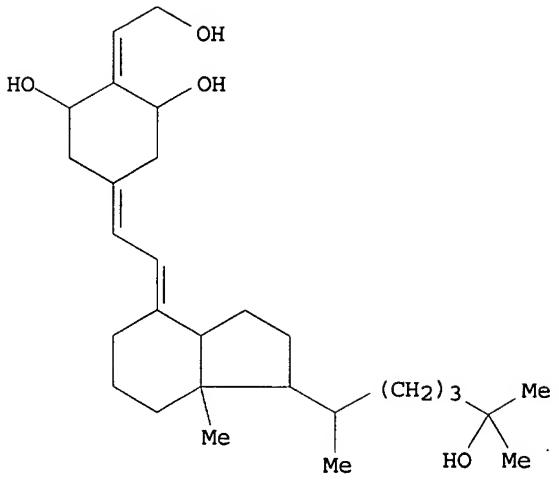
substituent at C(2) into 1α,25-dihydroxy-19-norvitamin D3 (2a) caused dramatic changes in binding affinity for the vitamin D receptor (VDR) and in transcriptional activity compared with the parent compound To investigate the broad biol. activity of 2-substituted 19-norvitamin D analogs, we synthesized two new (20S)-2-hydroxyethylidene-19-norvitaminD derivs. (3b and 4b) and a total of 16 A-ring-modified analogs including 3b and 4b were tested for the following in vitro and in vivo biol. activities: (1) affinity for the VDR, (2) transcriptional activity, (3) osteoclast formation, (4) bone calcium mobilization in rats, and (5) effects on differentiation of dendritic cells (DCs). The biol. effects of the analogs were compared with those of 1α,25-dihydroxyvitamin D3 (1a) and 2MD, which is being developed for the treatment of osteoporosis. The efficacy of the (20S)-19-norvitamin D analogs with 2-hydroxyethylidene, 2-hydroxyethoxy, and 2-Me moieties (3b, 5b, 6b, and 9b) was more than 10-fold stronger than that of 1a with respect to transcriptional activity, ability to induce osteoclast formation, and ability to inhibit CD86 expression, a marker of mature DCs, and was similar to that of 2MD. The (20S)-2β-hydroxyethoxy derivative 6b was 2 orders of magnitude more active than 1a and approx. twice as potent as 2MD in preventing CD86 production The 2-epoxy derivs. 7 and 8 were relatively poor ligands for the VDR and exhibited activity lower than that of the natural hormone 1a.

IT **681830-60-4P 681830-61-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

RN 681830-60-4 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)

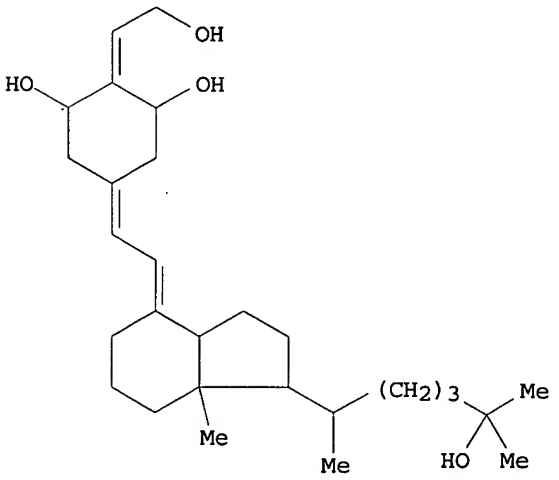


RN 681830-61-5 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)

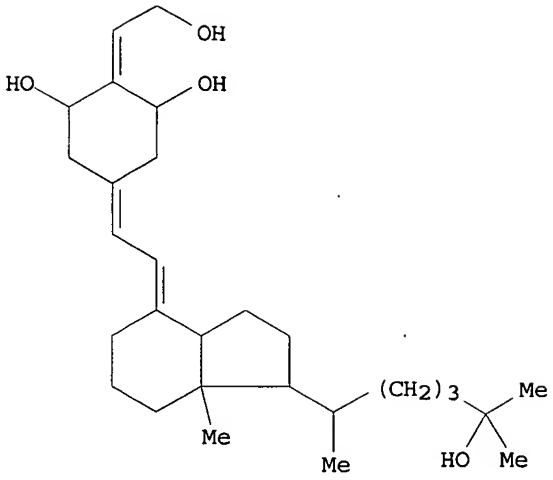


IT **737757-31-2 897923-11-4**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

RN 737757-31-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)

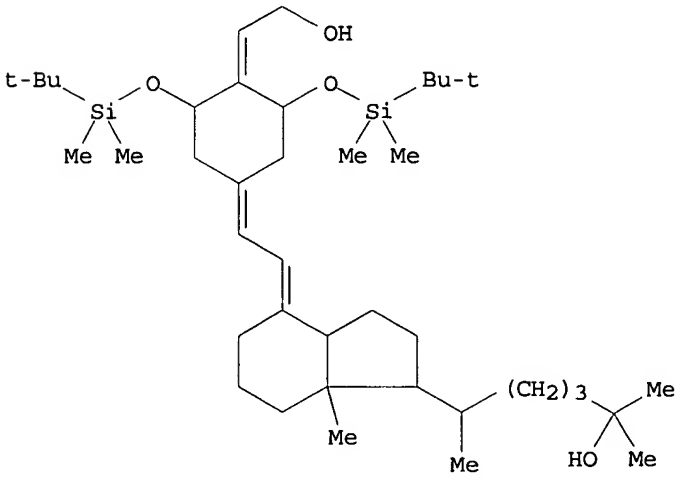


RN 897923-11-4 HCAPLUS
CN 1,3-Cyclohexanediol, 2-(2-hydroxyethylidene)-5-[[(1S,3aS,7aS)-octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,2S,3R)- (9CI) (CA INDEX NAME)

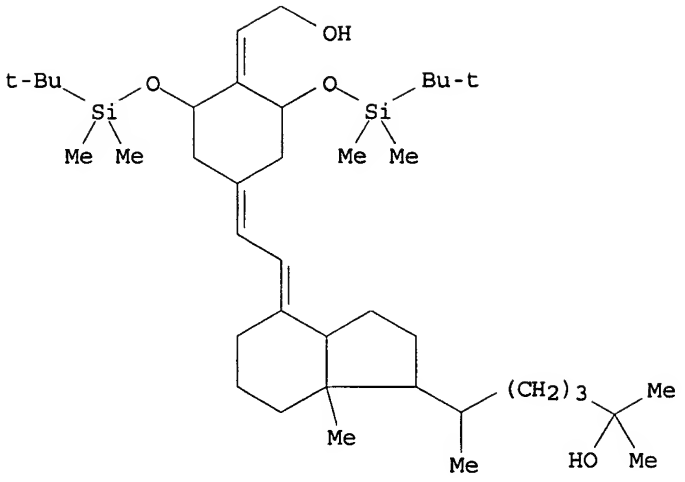


IT **681831-02-7P 681856-69-9P 900181-62-6P 900181-63-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

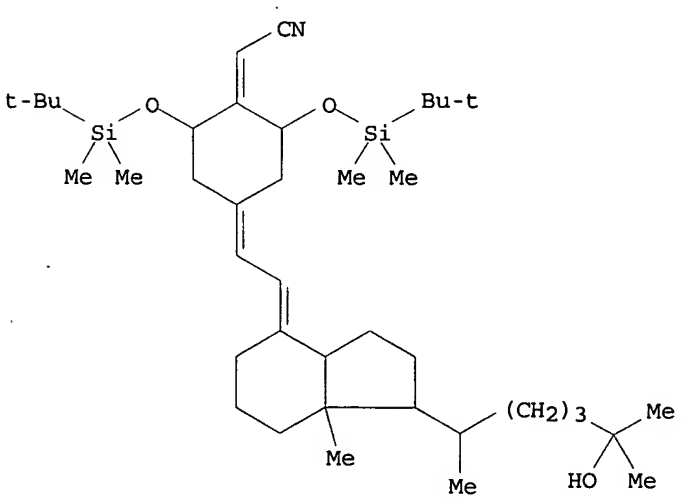
RN 681831-02-7 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-dien-25-ol,1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)



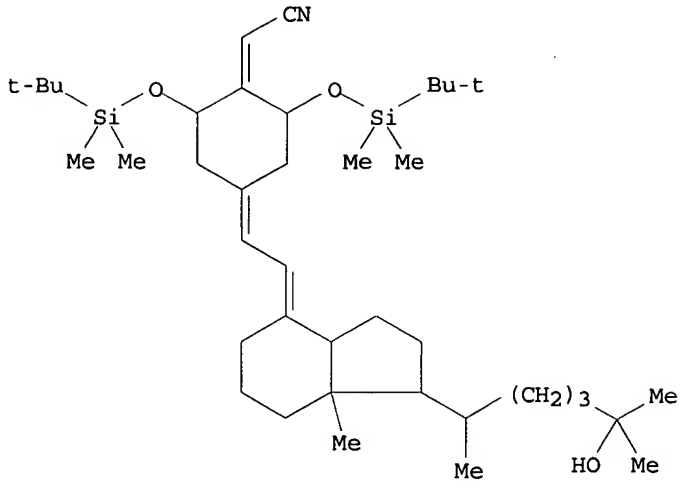
RN 681856-69-9 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-dien-25-ol,1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-(hydroxyethylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



RN 900181-62-6 HCAPLUS
CN Acetonitrile, [(1α,3β,7E,20S)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-hydroxy-19-nor-9,10-secocholesta-5,7-dien-2-ylidene]-, (2E)- (9CI) (CA INDEX NAME)



RN 900181-63-7 HCAPLUS
CN Acetonitrile, [(1α,3β,7E,20S)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-hydroxy-19-nor-9,10-secocholesta-5,7-dien-2-ylidene]-, (2Z)- (9CI) (CA INDEX NAME)



CC 1-3 (Pharmacology)
Section cross-reference(s): 2, 32

IT **681830-60-4P 681830-61-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

IT 32222-06-3 130447-37-9 134523-84-5 195051-26-4 546095-46-9 546100-84-9 681433-59-0 681830-46-6 681830-47-7 681830-58-0 681830-59-1 681830-95-5 681830-96-6 681856-65-5 **737757-31-2** 849816-81-5 849915-28-2 **897923-11-4**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

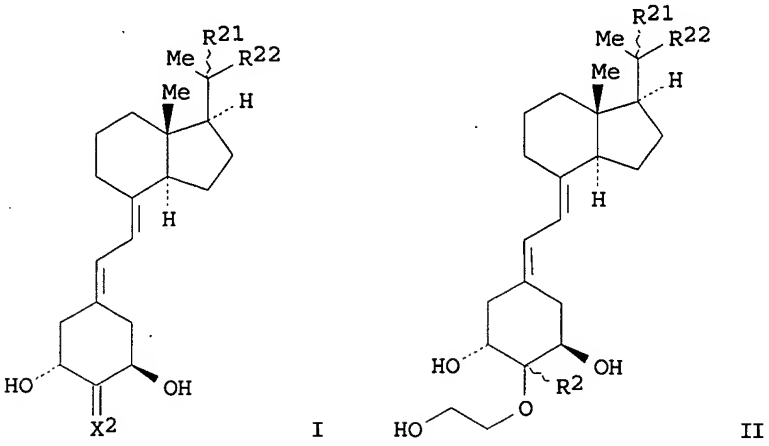
IT 681433-76-1P 681830-99-9P 681831-00-5P **681831-02-7P** **681856-69-9P** 681857-03-4P **900181-62-6P** **900181-63-7P** 903900-67-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dihydroxyvitamin D3 analogs with potency in induction of osteoclastogenesis and prevention of dendritic cell differentiation)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:447143 HCAPLUS
DOCUMENT NUMBER: 145:124780
TITLE: Synthesis and biological activities of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain
AUTHOR(S): Shimizu, Masato; Miyamoto, Yukiko; Kobayashi, Emi; Shimazaki, Mika; Yamamoto, Keiko; Reischl, Wolfgang; Yamada, Sachiko
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, School of Biomedical Science, Tokyo Medical and Dental University, 2-3-10 Kandasurugadai, Chiyoda-ku,

Tokyo, 101-0062, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(12), 4277-4294
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124780

GI

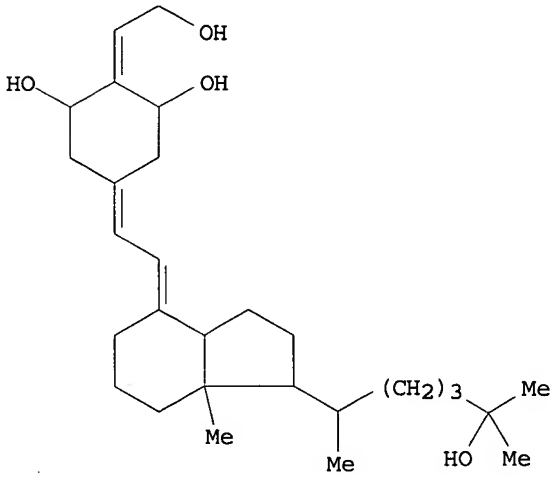


AB In a series of studies on structure-activity relationships of 2-substituted 19-norvitamin D analogs, we found that 1α,25-dihydroxy-19-norvitamin D3 analogs with 2β-hydroxyethoxy or 2E-hydroxyethylidene moieties show strong binding affinity for the vitamin D receptor (VDR) as well as marked transcriptional activity. To further examine the effects of side chain structure on the activity of 2-substituted 19-norvitamin D analogs, we have synthesized new 19-norvitamin D3 analogs with modifications in both the A-ring at the C(2) position and the side chain. The side chains of these analogs contained a double bond between C(22) and C(23) or an oxygen atom at C(22). The biol. activity of the analogs was evaluated in vitro. All the side chain-modified analogs were less active than 1α,25-dihydroxyvitamin D3 and the parent compds. I [X2 = CHCH2OH-(E), -(Z), R21 = β-H, R22 = (CH2)3CMe2OH] and II [R2 = α-, β-H, R21 = β-H, R22 = (CH2)3CMe2OH] possessing a natural 20R-configuration in binding to the VDR, but, except for the (20R)-22-oxa analogs I [X2 = CHCH2OH-(E), -(Z), R21 = α-H, R22 = O(CH2)2CMe2OH] and II [R2 = α-, β-H, R21 = α-H, R22 = O(CH2)2CMe2OH], were significantly more potent in transcriptional activity. Of the side-chain-modified analogs the 2β-hydroxyethoxy- and 2E-hydroxyethylidene-22,24-diene-24a,26a,27a-trihomo analogs showed markedly higher transcriptional activity (25- and 17.5-fold, resp.) compared with 1α,25-dihydroxyvitamin D3. Elongation of the side chain at the C-24, C-26, and C-27 positions and introduction of a 22,24-diene moiety strongly increased transcriptional activity, as seen in the 20-epi analogs I [X2 = CHCH2OH-(E), -(Z), R21 = α-H, R22 = (CH2)3CMe2OH] and II [R2 = α-, β-H, R21 = α-H, R22 = (CH2)3CMe2OH].

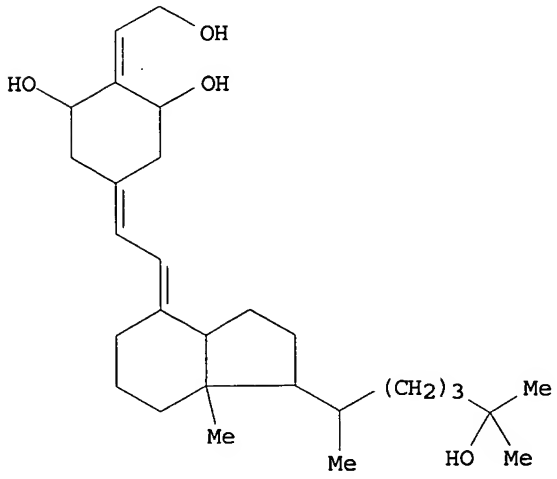
IT **681830-60-4 681830-61-5 737757-31-2 897923-11-4**
RL: PAC (Pharmacological activity); BIOL (Biological study)

(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)

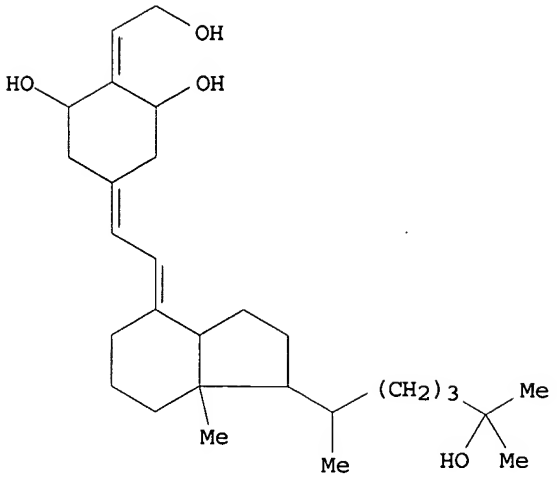
RN 681830-60-4 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)



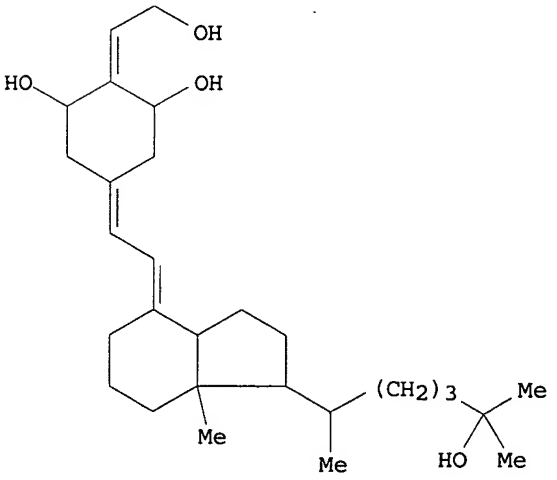
RN 681830-61-5 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



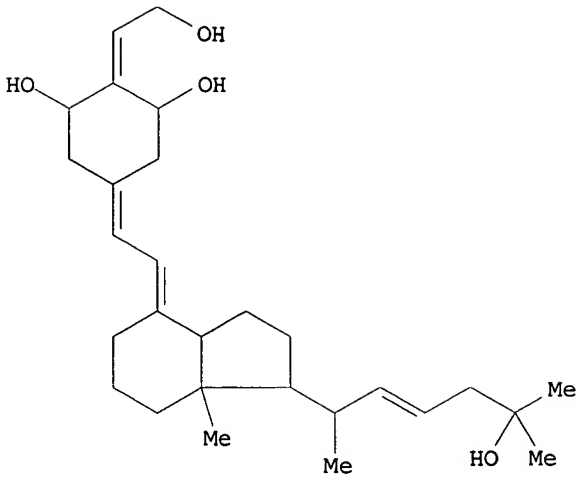
RN 737757-31-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)



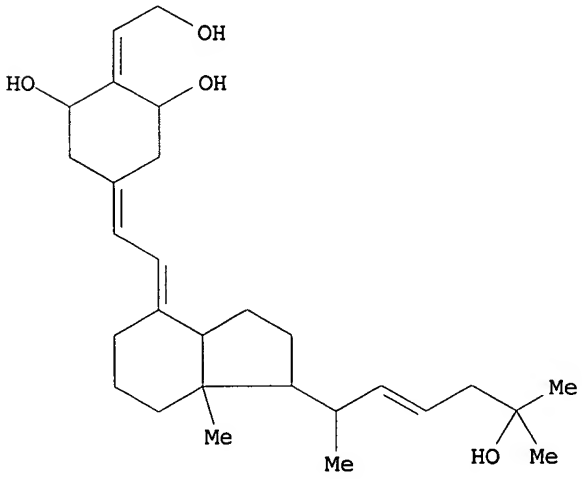
RN 897923-11-4 HCAPLUS
CN 1,3-Cyclohexanediol, 2-(2-hydroxyethylidene)-5-[[(1S,3aS,7aS)-octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,2S,3R)- (9CI) (CA INDEX NAME)



IT **681830-66-0P 681830-67-1P 681830-74-0P**
681830-75-1P 681830-84-2P 681830-85-3P
897923-07-8P 897923-08-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)
RN 681830-66-0 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7,22-triene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,22E)- (9CI) (CA INDEX NAME)



RN 681830-67-1 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7,22-triene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E,22E)- (9CI) (CA INDEX NAME)



RN 681830-74-0 HCAPLUS
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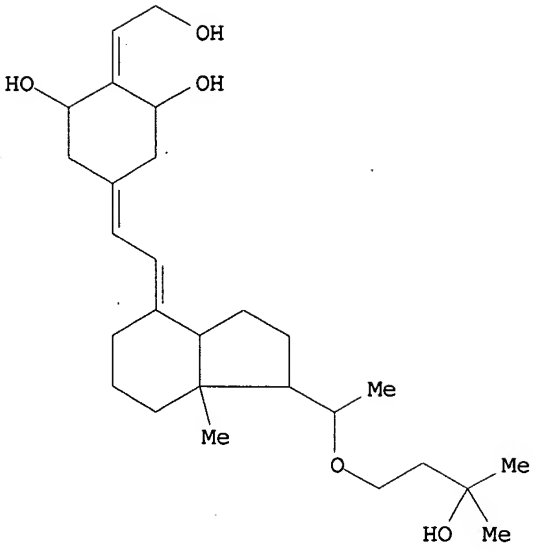

RN 681830-75-1 HCAPLUS
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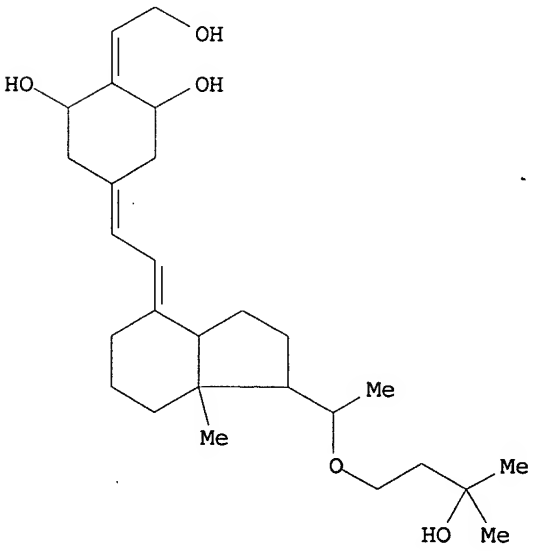

RN 681830-84-2 HCAPLUS
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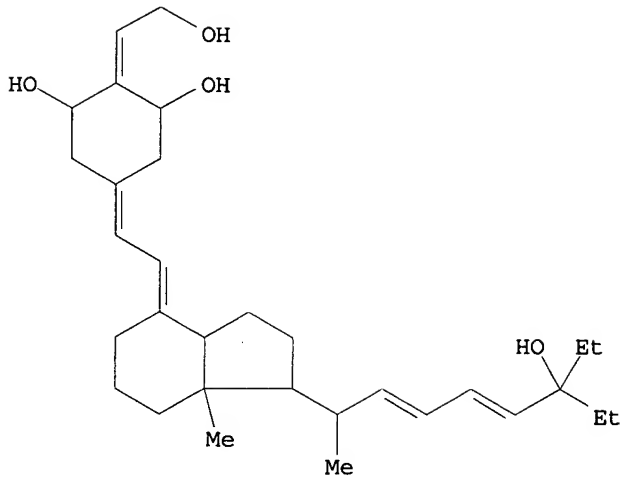

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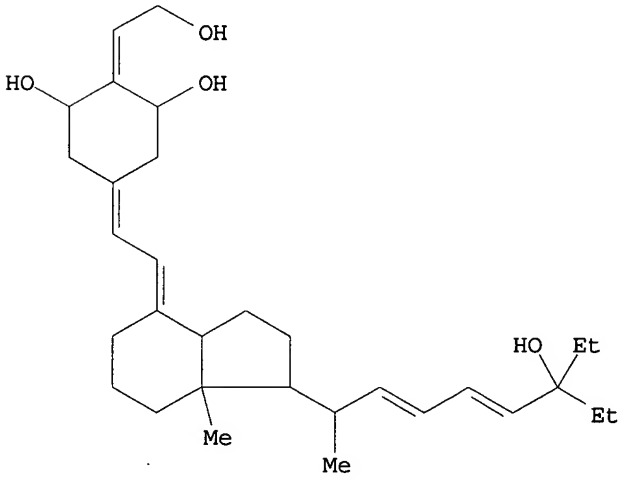

RN 897923-07-8 HCAPLUS
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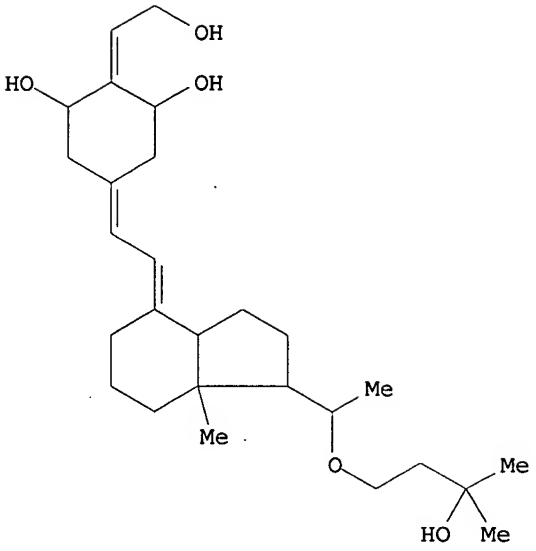
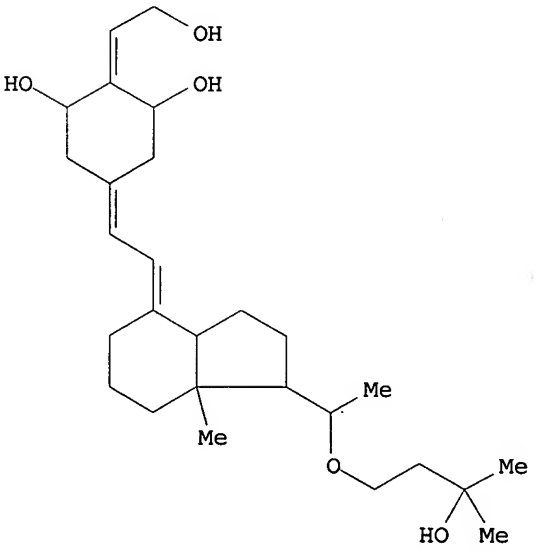


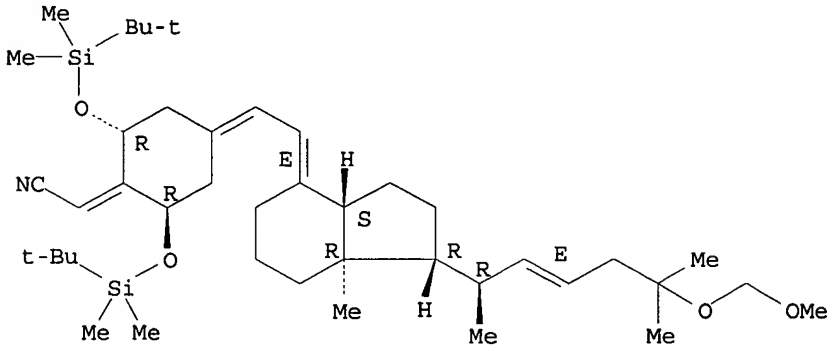
RN 897923-08-9 HCAPLUS
CN 1,3-Cyclohexanediol, 2-(2-hydroxyethylidene)-5-[(2E)-[(1S,3aS,7aS)-octahydro-1-[(1S)-1-(3-hydroxy-3-methylbutoxy)ethyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,2Z,3R)- (9CI) (CA INDEX NAME)



IT **681434-05-9P 681434-06-0P 681434-13-9P**
681434-14-0P 681831-07-2P 681831-08-3P
681831-10-7P 681856-70-2P 681856-71-3P
897657-90-8P 897657-91-9P 897657-92-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)
RN 681434-05-9 HCAPLUS
CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1R,3aS,7aR)-octahydro-1-[(1R,2E)-5-(methoxymethoxy)-1,5-dimethyl-2-hexenyl]-7a-methyl-4H-inden-4-

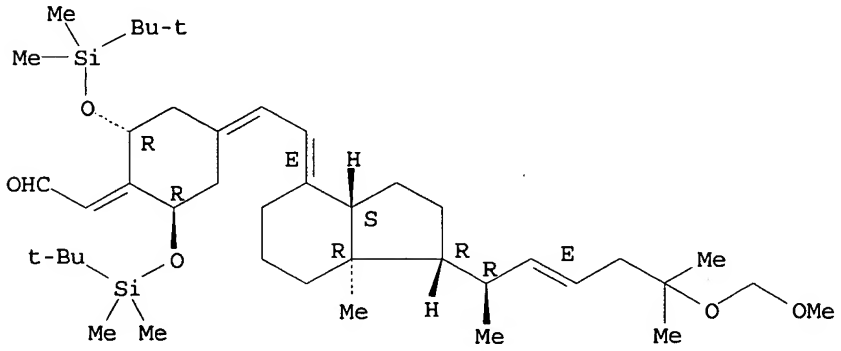
ylidene]ethylidene]cyclohexylidene]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



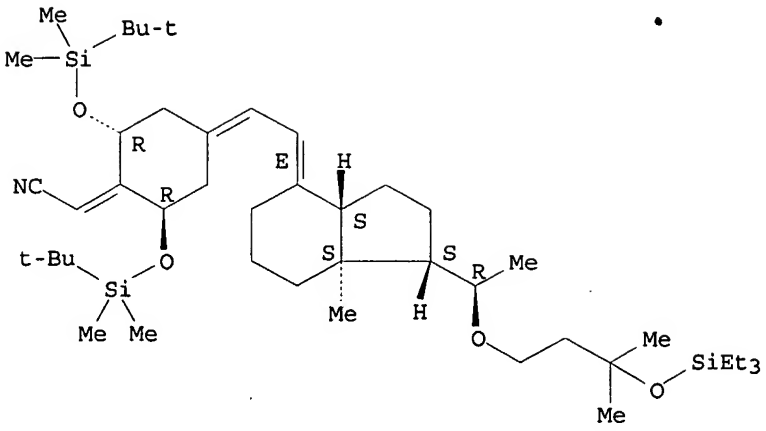
RN 681434-06-0 HCAPLUS
CN Acetaldehyde, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1R,3aS,7aR)-octahydro-1-[(1R,2E)-5-(methoxymethoxy)-1,5-dimethyl-2-hexenyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



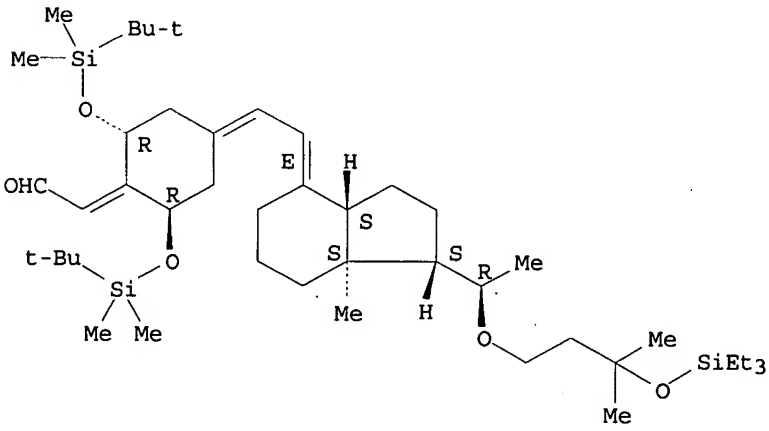
RN 681434-13-9 HCAPLUS
CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-7a-methyl-1-[(1R)-1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

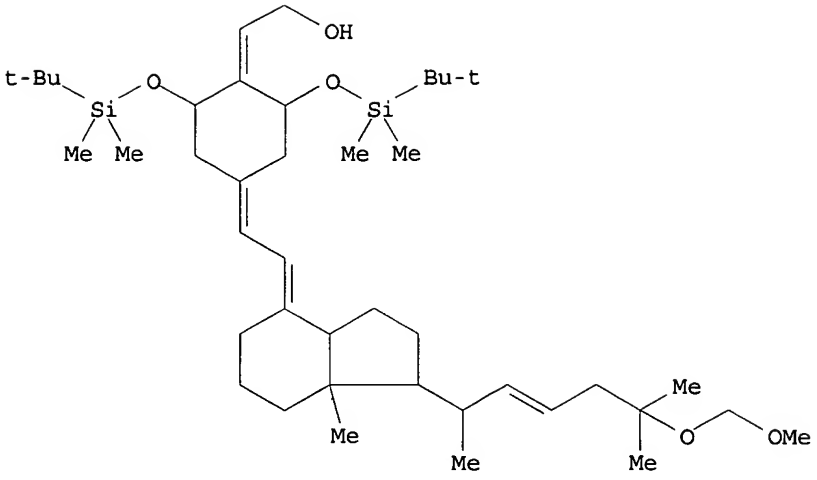


RN 681434-14-0 HCAPLUS
CN Acetaldehyde, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-7a-methyl-1-[(1R)-1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

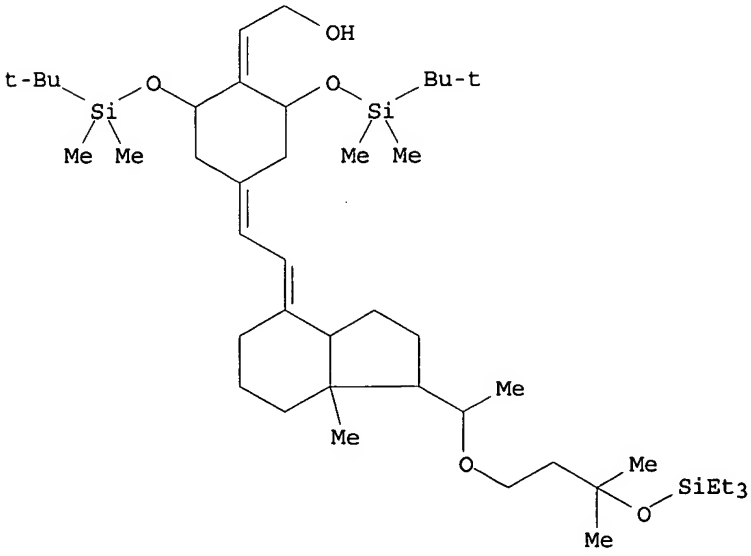
Absolute stereochemistry.
Double bond geometry as shown.



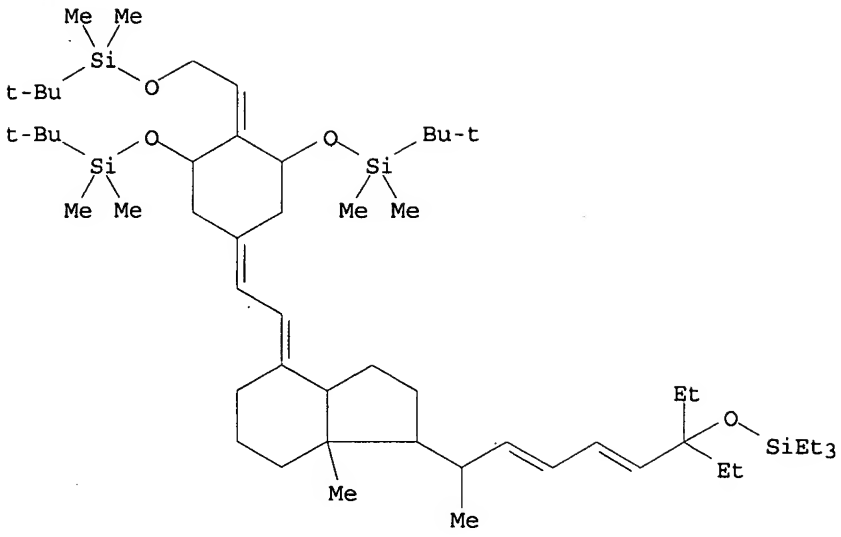
RN 681831-07-2 HCAPLUS
CN Ethanol, 2-[(1α,3β,7E,22E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7,22-trien-2-ylidene]-, (2E)- (9CI) (CA INDEX NAME)



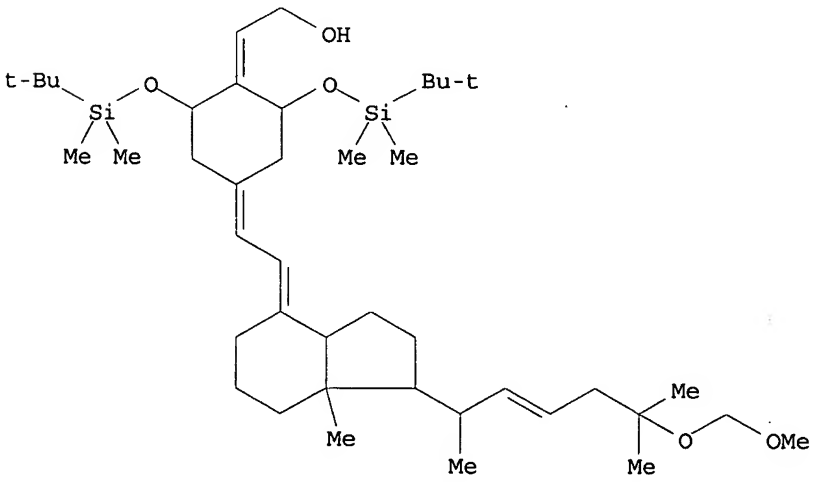
RN 681831-08-3 HCAPLUS
CN Ethanol, 2-[2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[[octahydro-7a-methyl-1-[1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-, stereoisomer (9CI) (CA INDEX NAME)



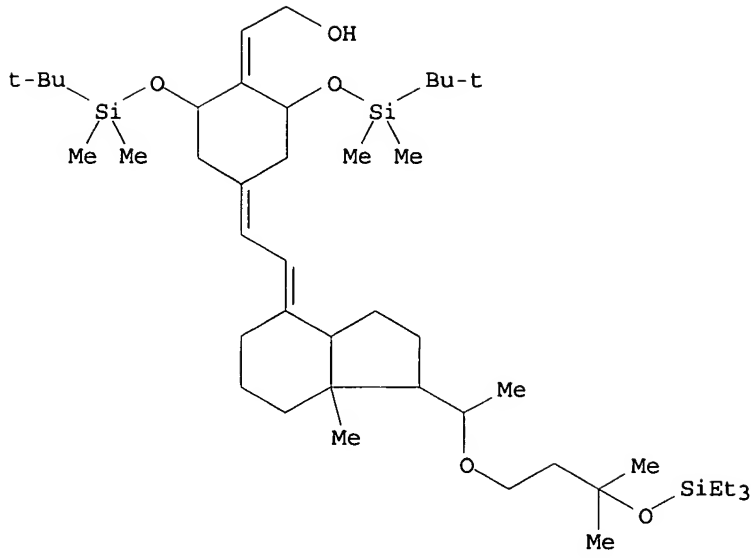
RN 681831-10-7 HCAPLUS
CN Silane, [[(1R,3R)-2-[(1E)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethylidene]-5-[(2E)-[(1R,3aS,7aR)-1-[(1R,2E,4E)-6-ethyl-1-methyl-6-[(triethylsilyl)oxy]-2,4-octadienyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-1,3-cyclohexanediyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



RN 681856-70-2 HCAPLUS
CN Ethanol, 2-[(1α,3β,7E,22E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7,22-trien-2-ylidene]-, (2Z)- (9CI) (CA INDEX NAME)

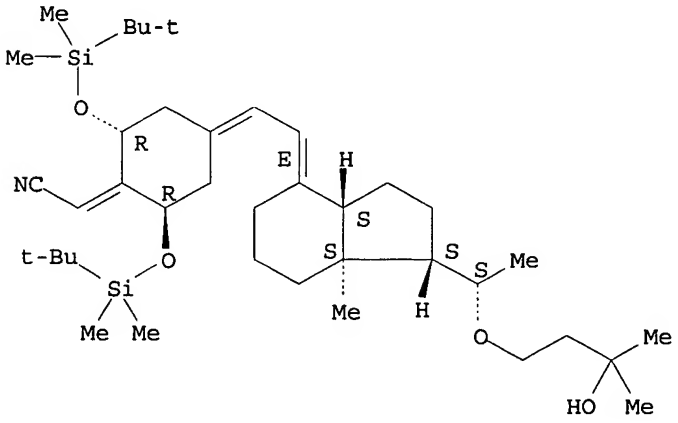


RN 681856-71-3 HCAPLUS
CN Ethanol, 2-[2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[[octahydro-7a-methyl-1-[1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-, stereoisomer (9CI) (CA INDEX NAME)



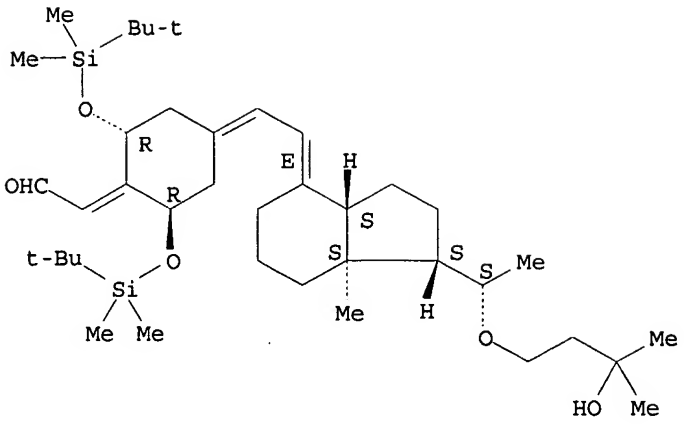
RN 897657-90-8 HCAPLUS
CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-1-[(1S)-1-(3-hydroxy-3-methylbutoxy)ethyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



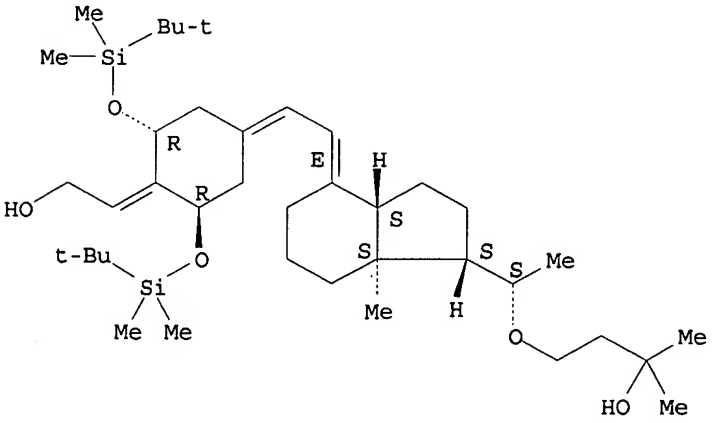
RN 897657-91-9 HCAPLUS
CN Acetaldehyde, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-1-[(1S)-1-(3-hydroxy-3-methylbutoxy)ethyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 897657-92-0 HCAPLUS
CN 2-Butanol, 4-[(1S)-1-[(1S,3aS,4E,7aS)-4-[[(3R,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-(2-hydroxyethylidene)cyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]ethoxy]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 32-7 (Steroids)
Section cross-reference(s): 1
IT 32222-06-3, 1α,25-Dihydroxyvitamin D3 546095-46-9
546100-84-9 681830-58-0 681830-59-1 **681830-60-4**
681830-61-5 737757-31-2 897923-11-4
RL: PAC (Pharmacological activity); BIOL (Biological study)
(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)
IT 67-97-0DP, Cholecalciferol, analogs 681830-64-8P 681830-65-9P
681830-66-0P 681830-67-1P 681830-72-8P
681830-73-9P **681830-74-0P 681830-75-1P**
681830-82-0P 681830-83-1P **681830-84-2P**
681830-85-3P 897923-07-8P 897923-08-9P
897923-09-0P 897923-10-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)

IT 2568-33-4P 17689-66-6P 192573-37-8P 681433-60-3P
681433-62-5P 681433-78-3P 681433-79-4P 681433-80-7P
681433-81-8P 681433-91-0P 681433-92-1P 681433-93-2P
681433-94-3P 681433-95-4P 681433-98-7P 681433-99-8P
681434-00-4P 681434-01-5P 681434-02-6P 681434-03-7P
681434-04-8P **681434-05-9P** **681434-06-0P**
681434-08-2P 681434-09-3P 681434-10-6P 681434-11-7P
681434-12-8P **681434-13-9P** **681434-14-0P**
681434-16-2P 681434-17-3P 681434-18-4P 681434-19-5P
681434-22-0P 681830-90-0P 681830-91-1P 681830-92-2P
681831-07-2P **681831-08-3P** **681831-10-7P**
681856-70-2P **681856-71-3P** 884488-07-7P
897657-83-9P 897657-84-0P 897657-85-1P 897657-86-2P
897657-87-3P 897657-88-4P 897657-89-5P **897657-90-8P**
897657-91-9P **897657-92-0P** 897923-05-6P
897923-06-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and vitamin D receptor binding activity of new 1α,25-dihydroxy-19-norvitamin D3 analogs with modifications in both the A-ring and the side chain)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

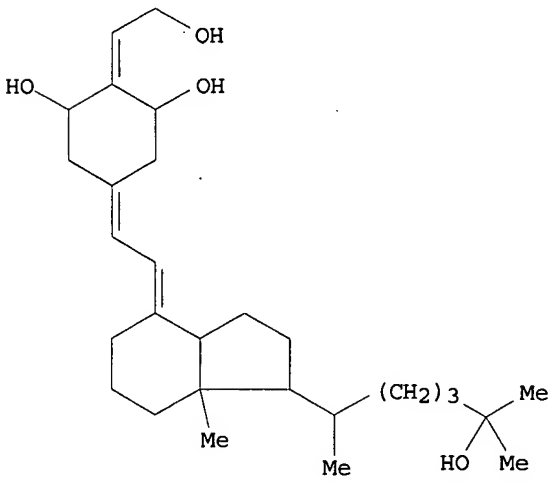
L19 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:522172 HCAPLUS
DOCUMENT NUMBER: 141:185222
TITLE: Two-dimensional alanine scanning mutational analysis of the interaction between the vitamin D receptor and its ligands: studies of A-ring modified 19-norvitamin D analogs
AUTHOR(S): Shimizu, Masato; Yamamoto, Keiko; Mihori, Mika; Iwasaki, Yukiko; Morizono, Daisuke; Yamada, Sachiko
CORPORATE SOURCE: Institute of Biomaterial and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (2004), 89-90(1-5), 75-81
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: : Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To clarify the structure-function relationship (SFR) of vitamin D analogs in terms of their interaction with the vitamin D receptor (VDR), we have proposed a new approach, two-dimensional alanine scanning mutational anal. (2D-ASMA). In this paper, attention was focused on the interactions around the A-ring of vitamin D. For this purpose, we synthesized four new 2-substituted 19-norvitamin D derivs. (3-6). The VDR affinity (3-6: 1, 5, 2 and 1/140, resp.) and transcriptional activity (3-6: 10, 30, 2 and 0.3, resp.) of the four compds. were evaluated relative to 1,25-(OH)2D3 (5) (normalized to 1). Then, the transcriptional activities of wild-type and 18 mutant VDRs induced by the four compds. (3-6) were investigated. The results of this 18+4 2D-ASMA were presented as a patch table, and the effects of the mutations were analyzed in comparison with the natural hormone (1) and 2-methylene-19-nor-20-epi-1,25-(OH)2D3 (2MD, 2). Of the four A-ring analogs, the 2α-hydroxyethoxy derivative (3) showed striking differences in the pattern on the patch table. From the results, we suggest a docking mode of this compound (3) in which the A-ring adopts the α conformation.

IT **737757-31-2P**
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP

(Preparation)
(two-dimensional alanine scanning mutational anal. of interaction between the vitamin D receptor and its ligands: studies of A-ring modified 19-norvitamin D analogs)

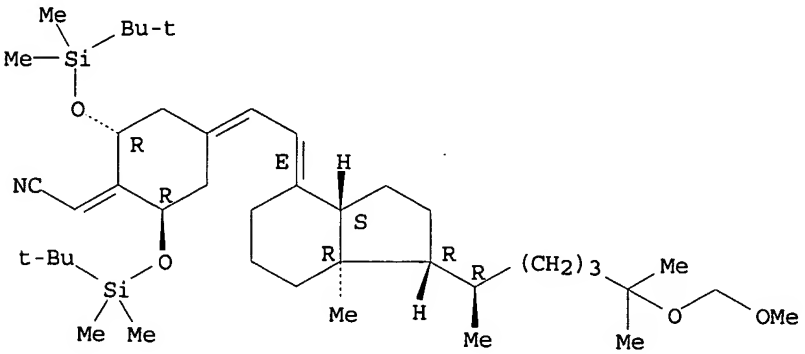
RN 737757-31-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E)- (9CI) (CA INDEX NAME)



IT **736982-52-8P 736982-53-9P 736982-54-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(two-dimensional alanine scanning mutational anal. of interaction between the vitamin D receptor and its ligands: studies of A-ring modified 19-norvitamin D analogs)

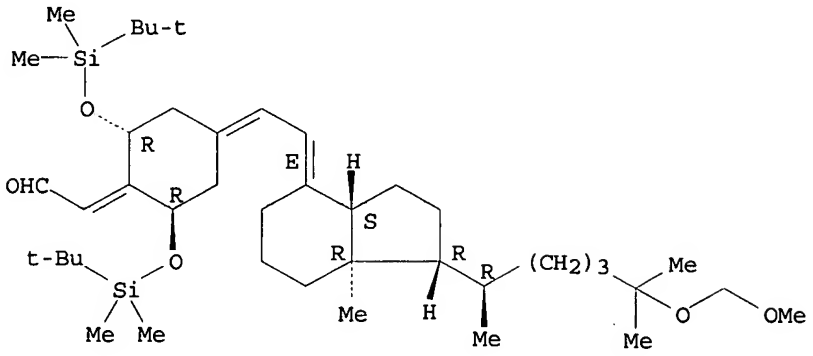
RN 736982-52-8 HCAPLUS
CN Acetonitrile, [(1α,3β,7E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7-dien-2-ylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



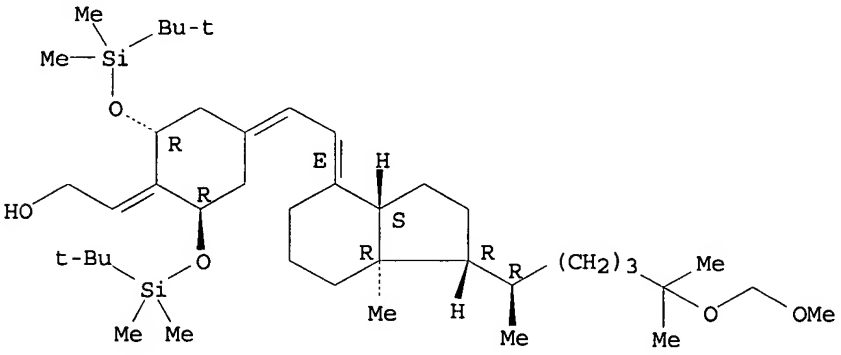
RN 736982-53-9 HCAPLUS
CN Acetaldehyde, [(1α,3β,7E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7-dien-2-ylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 736982-54-0 HCAPLUS
CN Ethanol, [(1α,3β,7E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7-dien-2-ylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 2-2 (Mammalian Hormones)
IT 681830-58-0P 681830-59-1P **737757-31-2P**
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(two-dimensional alanine scanning mutational anal. of interaction between the vitamin D receptor and its ligands: studies of A-ring modified 19-norvitamin D analogs)
IT 736982-50-6P 736982-51-7P **736982-52-8P**
736982-53-9P 736982-54-0P 737757-32-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(two-dimensional alanine scanning mutational anal. of interaction between the vitamin D receptor and its ligands: studies of A-ring modified 19-norvitamin D analogs)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:333691 HCAPLUS
DOCUMENT NUMBER: 140:357542
TITLE: Preparation of 2,2-di-substituted

1α,25-dihydroxy-19-norvitamin D derivatives as pharmaceuticals

INVENTOR(S): Yamada, Sachiko; Shimizu, Masato; Iwasaki, Yukiko

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

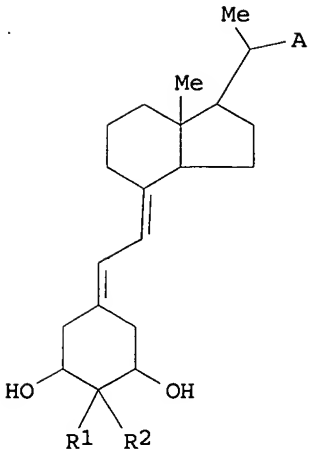
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004033420	A1	20040422	WO 2003-JP13053	2003 1010
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003271171	A1	20040504	AU 2003-271171	2003 1010
EP 1559708	A1	20050803	EP 2003-751451	2003 1010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006160779	A1	20060720	US 2005-530903	2005 0930

PRIORITY APPLN. INFO.:		
JP 2002-297366	A	2002 1010
JP 2003-24183	A	2003 0131
WO 2003-JP13053	W	2003 1010

OTHER SOURCE(S): MARPAT 140:357542

GI



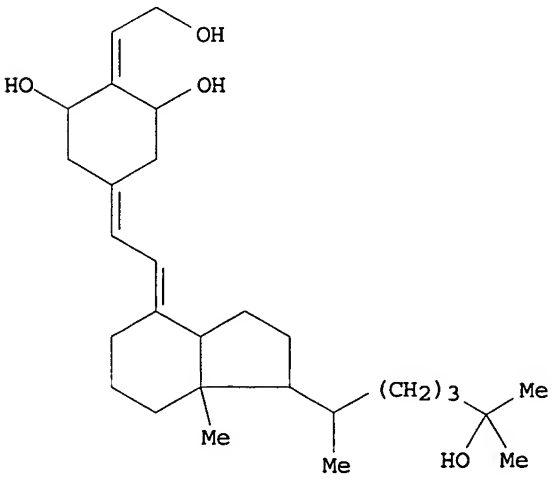
I

AB The title compds. I [R1 and R2 are the same or different and each represents hydroxy, etc.; and A represents hydrogen, unsubstituted linear or branched alkyl, etc.] are prepared The bioactivity of the title compds. was demonstrated. A process for preparing I is disclosed.

IT **681830-60-4P 681830-61-5P 681830-66-0P 681830-67-1P 681830-74-0P 681830-75-1P 681830-84-2P 681830-85-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,2-di-substituted 1α,25-dihydroxy-19-norvitamin D derivs. as pharmaceuticals)

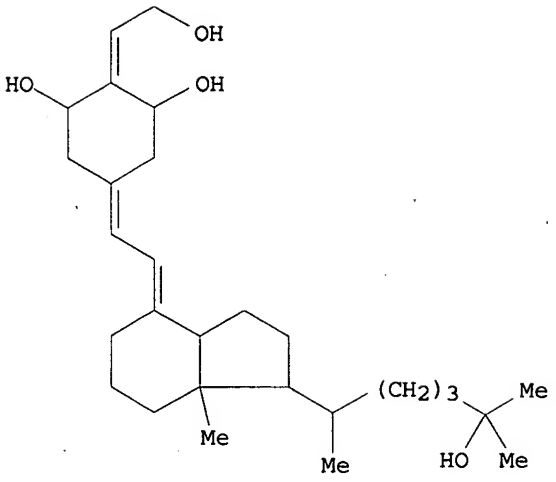
RN 681830-60-4 HCAPLUS

CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)

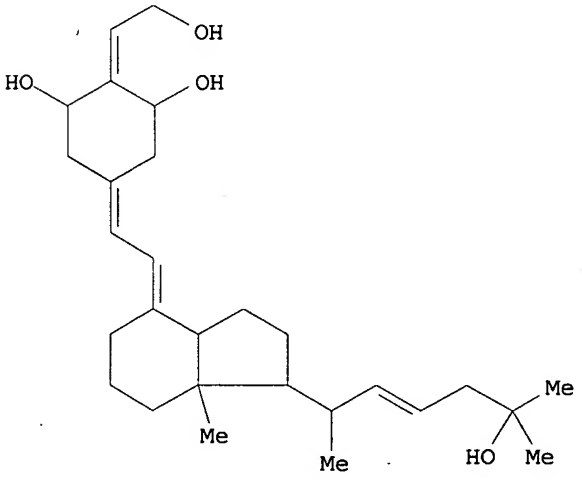


RN 681830-61-5 HCAPLUS

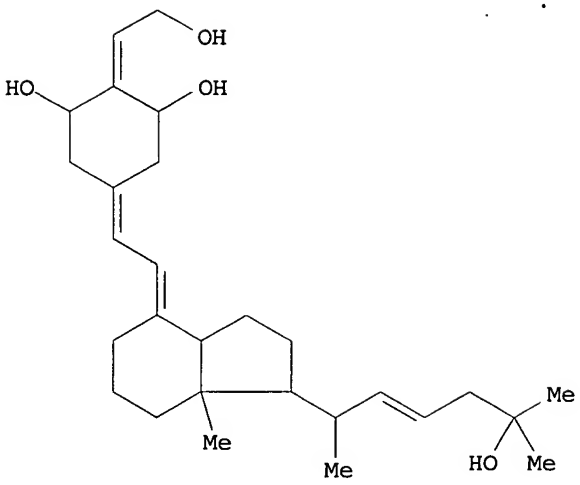
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



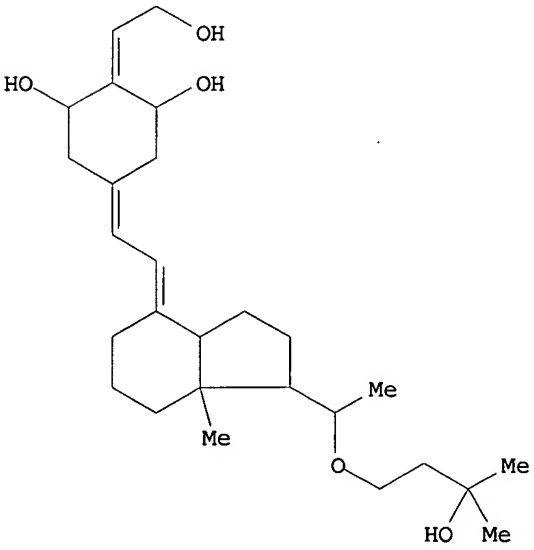
RN 681830-66-0 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7,22-triene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,22E)- (9CI) (CA INDEX NAME)



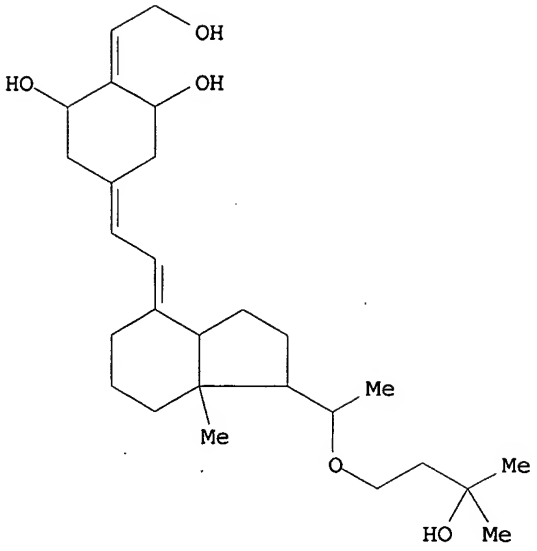
RN 681830-67-1 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7,22-triene-1,3,25-triol, 2-(2-hydroxyethylidene)-, (1α,2Z,3β,7E,22E)- (9CI) (CA INDEX NAME)



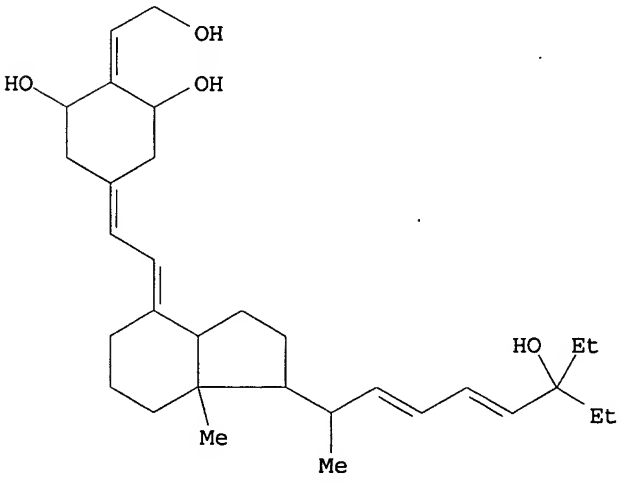
RN 681830-74-0 HCAPLUS
CN 1,3-Cyclohexanediol, 2-(2-hydroxyethylidene)-5-[[octahydro-1-[1-(3-hydroxy-3-methylbutoxy)ethyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, stereoisomer (9CI) (CA INDEX NAME)



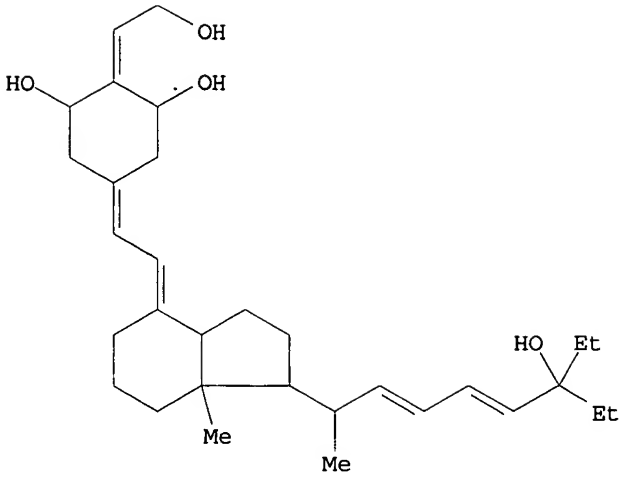
RN 681830-75-1 HCAPLUS
CN 1,3-Cyclohexanediol, 2-(2-hydroxyethylidene)-5-[[octahydro-1-[1-(3-hydroxy-3-methylbutoxy)ethyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, stereoisomer (9CI) (CA INDEX NAME)



RN 681830-84-2 HCAPLUS
CN 1,3-Cyclohexanediol, 5-[[1-(6-ethyl-6-hydroxy-1-methyl-2,4-octadienyl)octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-(2-hydroxyethylidene)-, stereoisomer (9CI) (CA INDEX NAME)



RN 681830-85-3 HCAPLUS
CN 1,3-Cyclohexanediol, 5-[[1-(6-ethyl-6-hydroxy-1-methyl-2,4-octadienyl)octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-(2-hydroxyethylidene)-, stereoisomer (9CI) (CA INDEX NAME)

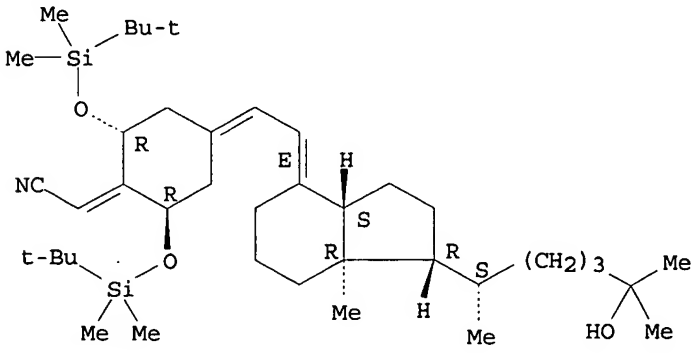


IT **681433-77-2P 681434-05-9P 681434-06-0P**
681434-13-9P 681434-14-0P 681831-02-7P
681831-07-2P 681831-08-3P 681831-10-7P
681856-69-9P 681856-70-2P 681856-71-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,2-di-substituted 1α,25-dihydroxy-19-norvitamin D derivs. as pharmaceuticals)

RN 681433-77-2 HCAPLUS

CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1R,3aS,7aR)-octahydro-1-[(1S)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

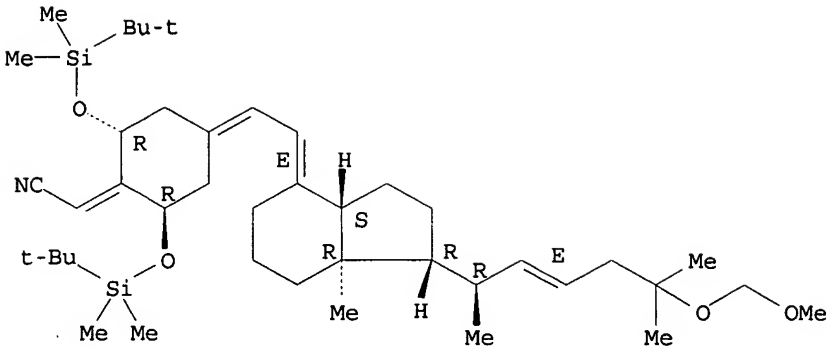
Absolute stereochemistry.
Double bond geometry as shown.



RN 681434-05-9 HCAPLUS

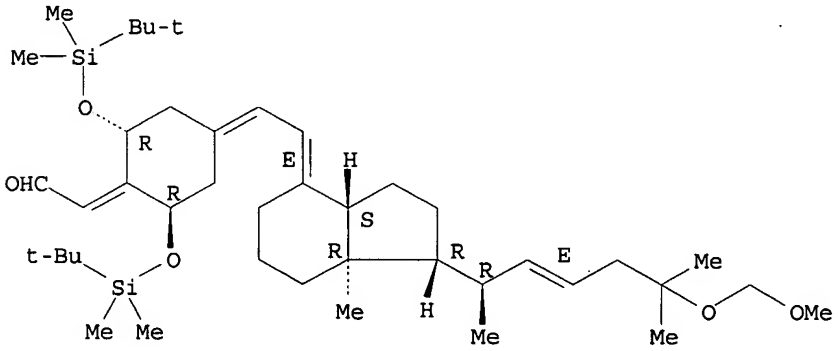
CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1R,3aS,7aR)-octahydro-1-[(1R,2E)-5-(methoxymethoxy)-1,5-dimethyl-2-hexenyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



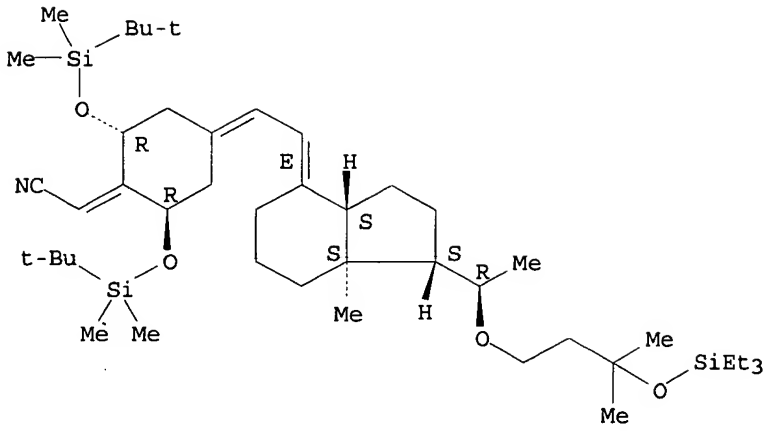
RN 681434-06-0 HCAPLUS
CN Acetaldehyde, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1R,3aS,7aR)-octahydro-1-[(1R,2E)-5-(methoxymethoxy)-1,5-dimethyl-2-hexenyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



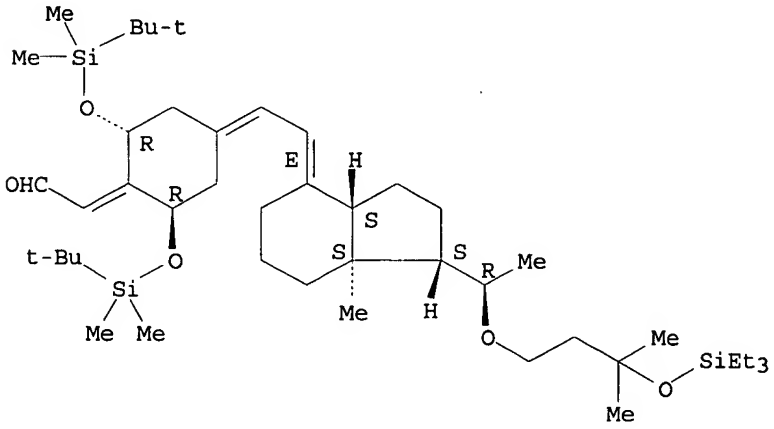
RN 681434-13-9 HCAPLUS
CN Acetonitrile, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-7a-methyl-1-[(1R)-1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

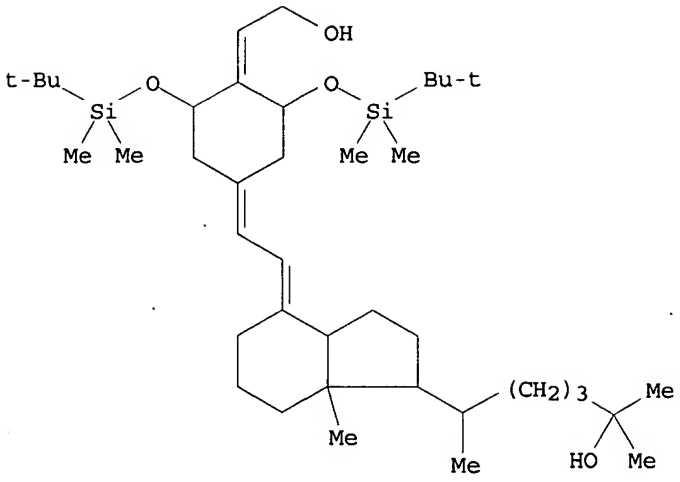


RN 681434-14-0 HCAPLUS
CN Acetaldehyde, [(2R,6R)-2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[(2E)-[(1S,3aS,7aS)-octahydro-7a-methyl-1-[(1R)-1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]- (9CI) (CA INDEX NAME)

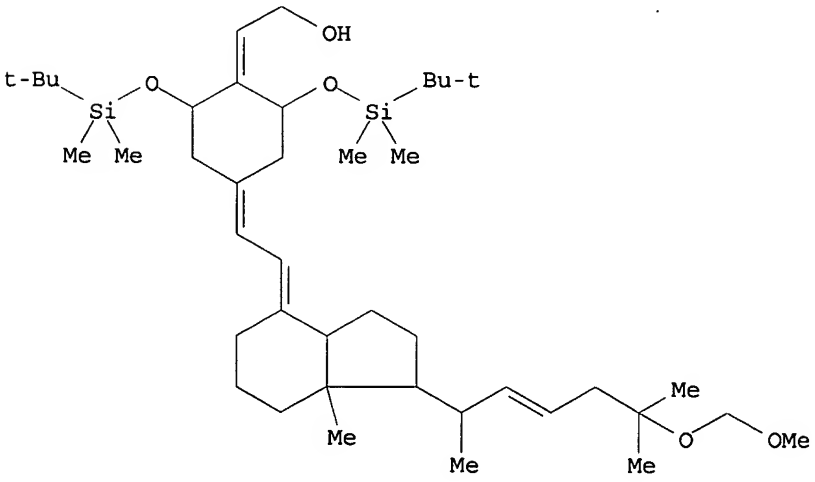
Absolute stereochemistry.
Double bond geometry as shown.



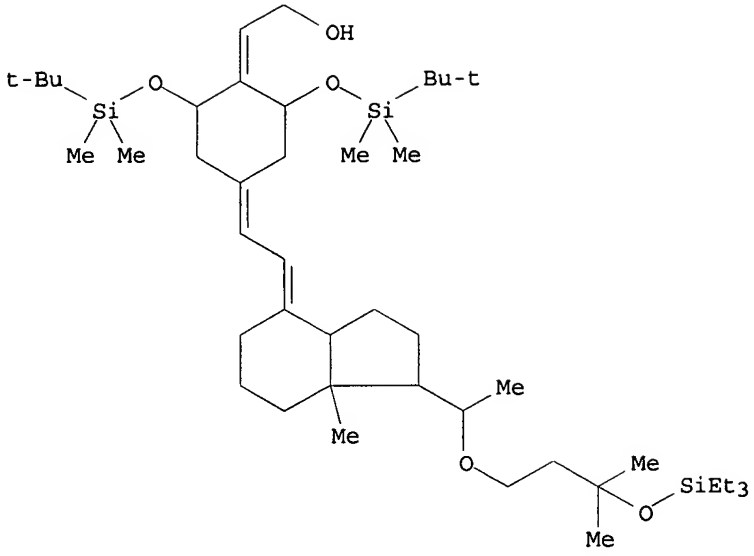
RN 681831-02-7 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-dien-25-ol,1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-(2-hydroxyethylidene)-, (1α,2E,3β,7E,20S)- (9CI) (CA INDEX NAME)



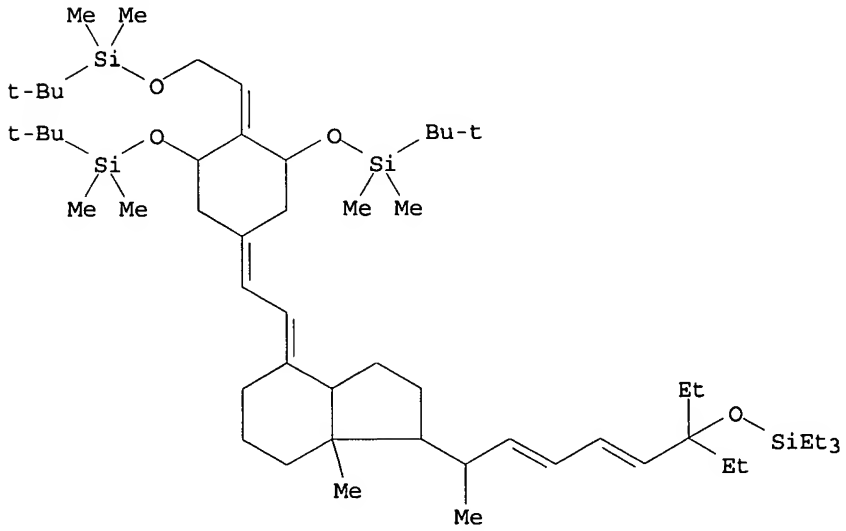
RN 681831-07-2 HCAPLUS
CN Ethanol, 2-[(1α,3β,7E,22E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7,22-trien-2-ylidene]-, (2E)- (9CI) (CA INDEX NAME)



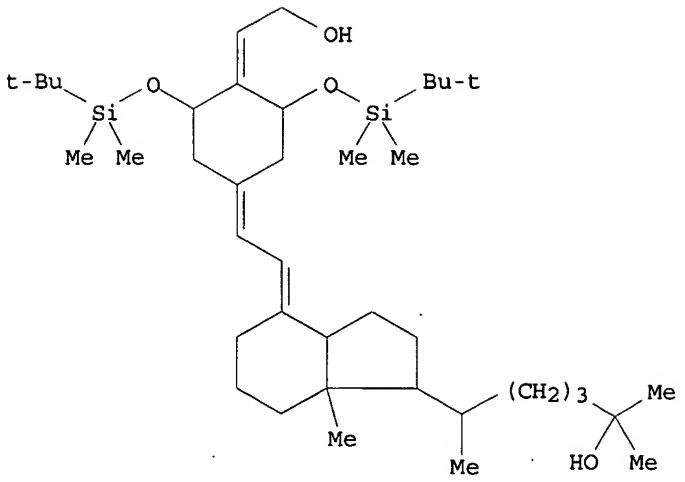
RN 681831-08-3 HCAPLUS
CN Ethanol, 2-[2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[[octahydro-7a-methyl-1-[1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-, stereoisomer (9CI) (CA INDEX NAME)



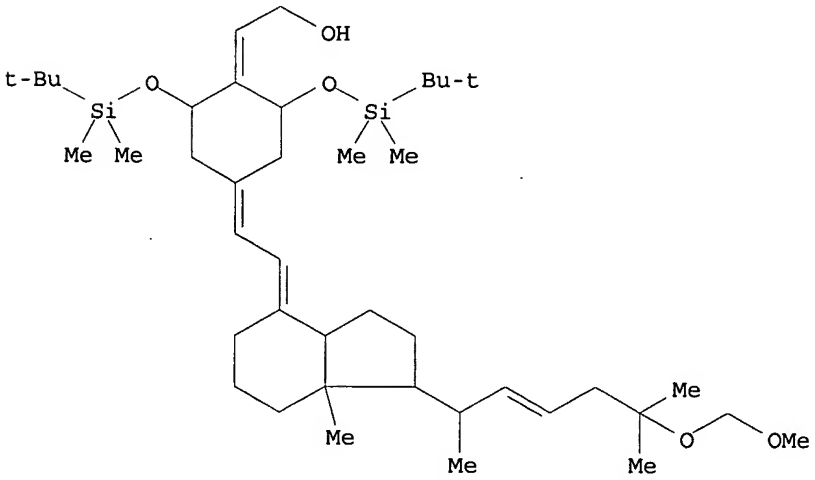
RN 681831-10-7 HCAPLUS
CN Silane, [[(1R,3R)-2-[(1E)-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethylidene]-5-[(2E)-[(1R,3aS,7aR)-1-[(1R,2E,4E)-6-ethyl-1-methyl-6-[(triethylsilyl)oxy]-2,4-octadienyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-1,3-cyclohexanediyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



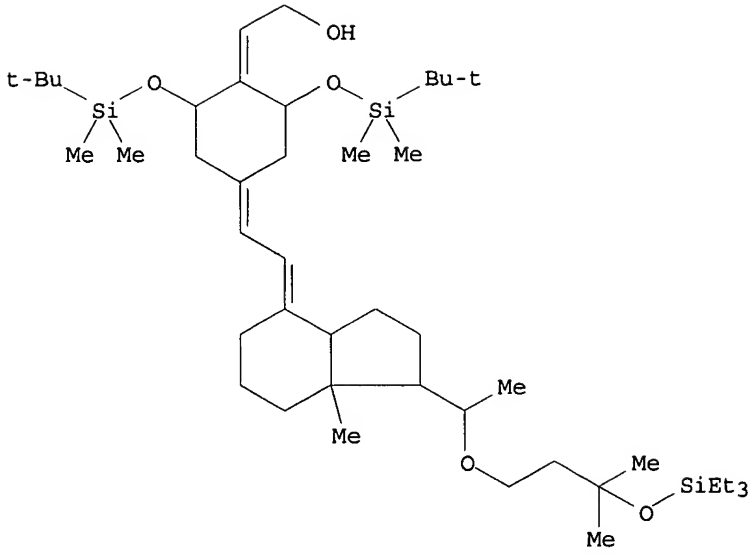
RN 681856-69-9 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-dien-25-ol,1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-(hydroxyethylidene)-, (1α,2Z,3β,7E,20S)- (9CI) (CA INDEX NAME)



RN 681856-70-2 HCAPLUS
CN Ethanol, 2-[(1α,3β,7E,22E)-1,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-25-(methoxymethoxy)-19-nor-9,10-secocholesta-5,7,22-trien-2-ylidene]-, (2Z)- (9CI) (CA INDEX NAME)



RN 681856-71-3 HCAPLUS
CN Ethanol, 2-[2,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-[[octahydro-7a-methyl-1-[1-[3-methyl-3-[(triethylsilyl)oxy]butoxy]ethyl]-4H-inden-4-ylidene]ethylidene]cyclohexylidene]-, stereoisomer (9CI) (CA INDEX NAME)



IC ICM C07C401-00
ICS A61K031-59; A61P035-00; A61P037-02; A61P043-00
CC 32-7 (Steroids)
Section cross-reference(s): 1, 63
IT 681433-59-0P 681433-60-3P 681830-46-6P 681830-47-7P
681830-48-8P 681830-49-9P 681830-50-2P 681830-51-3P
681830-52-4P 681830-53-5P 681830-55-7P 681830-56-8P
681830-57-9P 681830-58-0P 681830-59-1P **681830-60-4P**
681830-61-5P 681830-62-6P 681830-63-7P 681830-64-8P
681830-65-9P **681830-66-0P** **681830-67-1P**
681830-68-2P 681830-69-3P 681830-70-6P 681830-71-7P
681830-72-8P 681830-73-9P **681830-74-0P**
681830-75-1P 681830-76-2P 681830-77-3P 681830-78-4P
681830-79-5P 681830-80-8P 681830-81-9P 681830-82-0P
681830-83-1P **681830-84-2P** **681830-85-3P**
681830-86-4P 681830-87-5P 681830-88-6P 681830-89-7P
681830-95-5P 681830-96-6P 681856-65-5P 681856-66-6P
681856-67-7P 681857-01-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,2-di-substituted 1α,25-dihydroxy-19-norvitamin D derivs. as pharmaceuticals)
IT 139131-74-1P 139131-75-2P 139131-76-3P 147725-63-1P
681433-62-5P 681433-63-6P 681433-64-7P 681433-65-8P
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681433-71-6P 681433-72-7P 681433-73-8P 681433-74-9P
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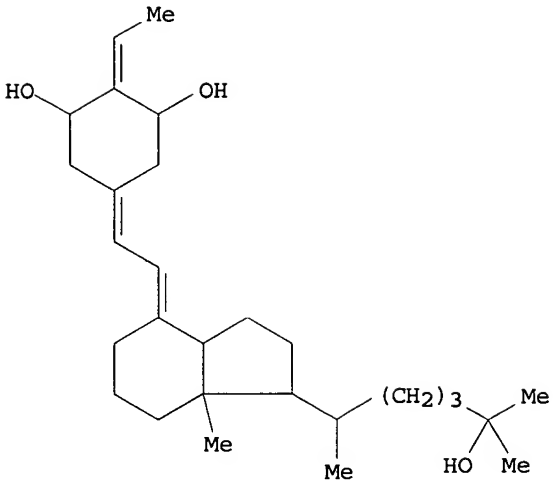
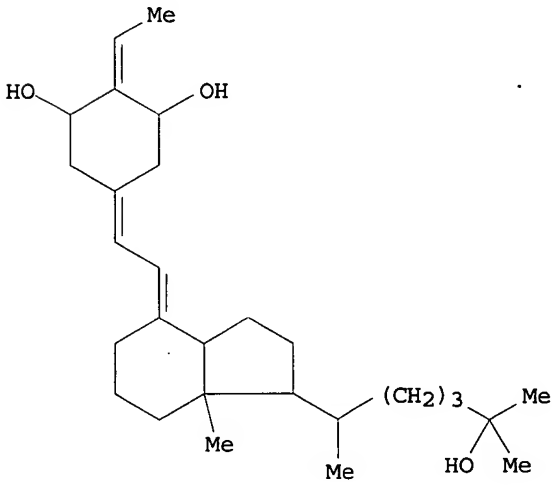
681831-08-3P 681831-09-4P **681831-10-7P**
681831-11-8P 681856-68-8P **681856-69-9P**
681856-70-2P **681856-71-3P** 681857-02-3P
681857-03-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,2-di-substituted 1α,25-dihydroxy-19-norvitamin D derivs. as pharmaceuticals)
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

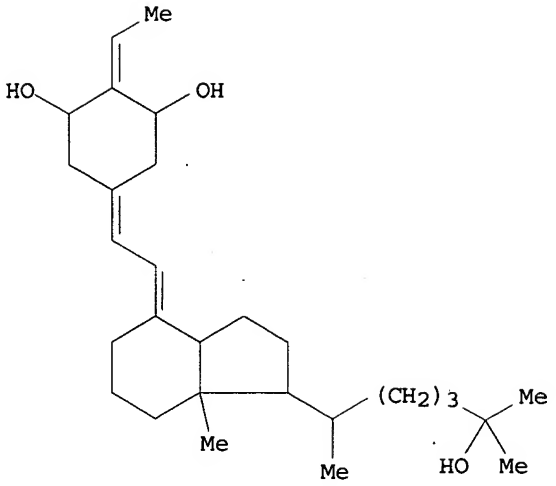
L19 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:485206 HCAPLUS
DOCUMENT NUMBER: 137:217136
TITLE: 2-Ethyl and 2-Ethylidene Analogues of 1α,25-Dihydroxy-19-norvitamin D3: Synthesis, Conformational Analysis, Biological Activities, and Docking to the Modeled rVDR Ligand Binding Domain
AUTHOR(S): Sicinski, Rafal R.; Rotkiewicz, Piotr; Kolinski, Andrzej; Sicinska, Wanda; Prahl, Jean M.; Smith, Connie M.; DeLuca, Hector F.
CORPORATE SOURCE: Department of Biochemistry, University of Wisconsin, Madison, WI, 53706, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3366-3380
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:217136
AB Novel 19-nor analogs of 1α,25-dihydroxyvitamin D3 were prepared and substituted at C-2 with an ethylidene group. The synthetic pathway was via Wittig-Horner coupling of the corresponding A-ring phosphine oxides with the protected 25-hydroxy Grundmann's ketones. Selective catalytic hydrogenation of 2-ethylidene analogs provided the 2α- and 2β-Et compds. The 2-ethylidene-19-nor compds. with a Me group from the ethylidene moiety in a trans relationship to the C(6)-C(7) bond (E-isomers) were more potent than the corresponding Z-isomers and the natural hormone in binding to the vitamin D receptor. Both geometrical isomers (E and Z) of (20S)-2-ethylidene-19-norvitamin D3 and both 2α-ethyl-19-norvitamins (in the 20R- and 20S-series) have much higher HL-60 differentiation activity than does 1α,25-(OH)2D3. Both E-isomers (20R and 20S) of 2-ethylidene vitamins are characterized by very high calcemic activity in rats. The three-dimensional structure model of the rat vitamin D receptor and the computational docking of four synthesized (20R)-19-norvitamin D3 analogs into its binding pocket are also reported.
IT **377086-22-1P** **377086-23-2P** **377086-32-3P**
377087-90-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Et and ethylidene dihydroxy-19-norvitamin D3 analogs via Wittig-Horner, their conformation, vitamin D receptor activity, calcium transport and mobilization activities, and HL-60 differentiation)
RN 377086-22-1 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2E,3β)- (9CI) (CA INDEX NAME)



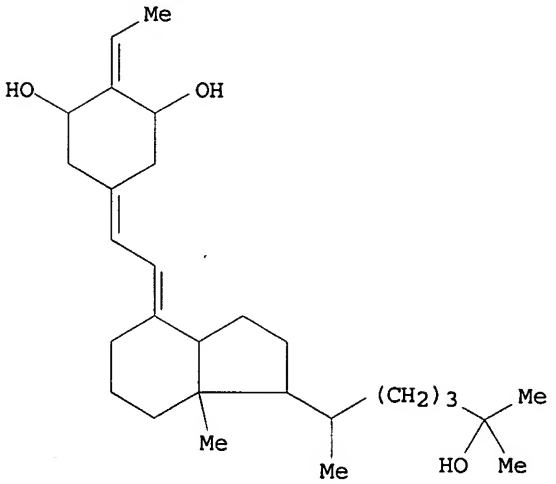
RN 377086-23-2 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2Z,3β)- (9CI) (CA INDEX NAME)



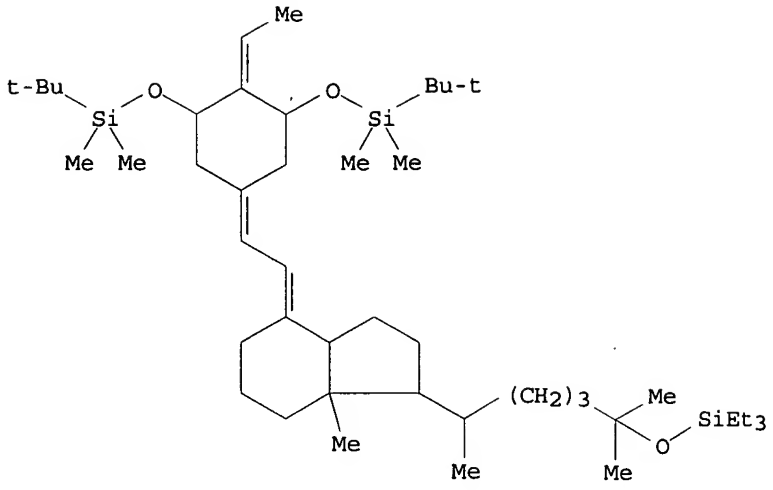
RN 377086-32-3 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2Z,3β,20S)- (9CI) (CA INDEX NAME)



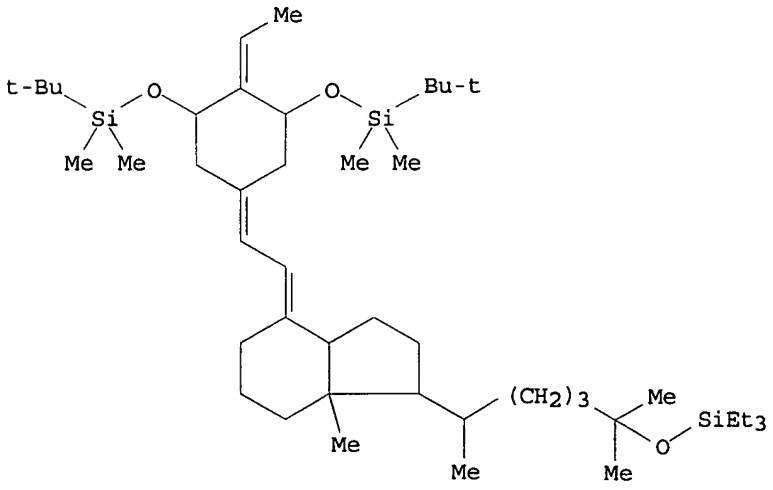
RN 377087-90-6 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2E,3β,20S)- (9CI) (CA INDEX NAME)



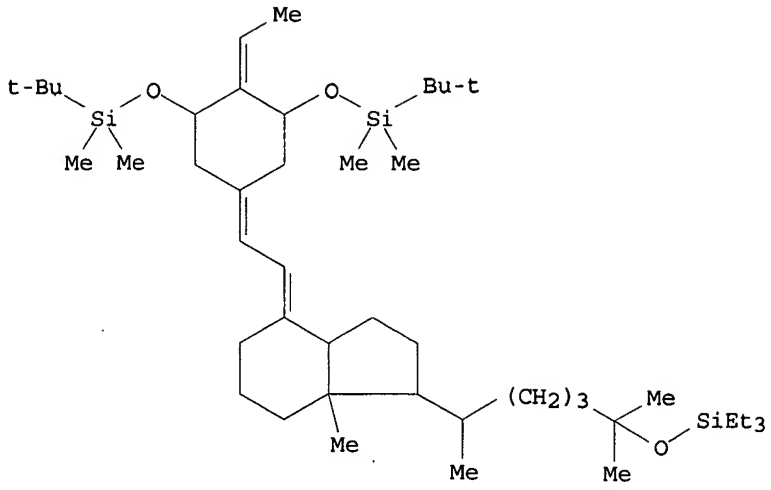
IT **377086-30-1P 455253-25-5P 455253-26-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Et and ethylidene dihydroxy-19-norvitamin D3 analogs via Wittig-Horner, their conformation, vitamin D receptor activity, calcium transport and mobilization activities, and HL-60 differentiation)
RN 377086-30-1 HCAPLUS
CN Silane, [[(1α,2E,3β,7E)-2-ethylidene-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



RN 455253-25-5 HCAPLUS
CN Silane, [[(1α,2E,3β,7E,20S)-2-ethylidene-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



RN 455253-26-6 HCAPLUS
CN Silane, [[(1α,2Z,3β,7E,20S)-2-ethylidene-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



CC 32-7 (Steroids)
Section cross-reference(s): 1
IT **377086-22-1P 377086-23-2P 377086-32-3P**
377087-90-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Et and ethylidene dihydroxy-19-norvitamin D3 analogs via Wittig-Horner, their conformation, vitamin D receptor activity, calcium transport and mobilization activities, and HL-60 differentiation)
IT 376353-72-9P 376353-73-0P 376353-74-1P 377086-26-5P
377086-27-6P 377086-28-7P 377086-29-8P **377086-30-1P**
455253-25-5P 455253-26-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Et and ethylidene dihydroxy-19-norvitamin D3 analogs via Wittig-Horner, their conformation, vitamin D receptor activity, calcium transport and mobilization activities, and HL-60 differentiation)
REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:886060 HCAPLUS
DOCUMENT NUMBER: 136:6208
TITLE: Preparation and formulation of 2-ethyl and 2-ethylidene-19-nor-vitamin D compounds
INVENTOR(S): Deluca, Hector F.; Sicinski, Rafal R.
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092221	A1	20011206	WO 2001-US17662	2001 0531

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2410880	AA	20011206	CA 2001-2410880	2001 0531
US 2003013691	A1	20030116	US 2001-871227	2001 0531
US 6806262	B2	20041019		
EP 1286962	A1	20030305	EP 2001-939792	2001 0531

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BR 2001011173	A	20030429	BR 2001-11173	2001 0531
JP 2004501114	T2	20040115	JP 2002-500836	2001 0531
NZ 522909	A	20040924	NZ 2001-522909	2001 0531
EP 1524264	A2	20050420	EP 2005-1268	2001 0531

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR

US 2005043281	A1	20050224	US 2004-957483	2004 1001
US 6992074	B2	20060131		
US 2005282789	A1	20051222	US 2005-191791	2005 0728

PRIORITY APPLN. INFO.:			US 2000-208199P	P 2000 0531
			EP 2001-939792	A3 2001 0531
			US 2001-871227	A 2001 0531
			WO 2001-US17662	W 2001 0531
			US 2004-957483	A3 2004 1001

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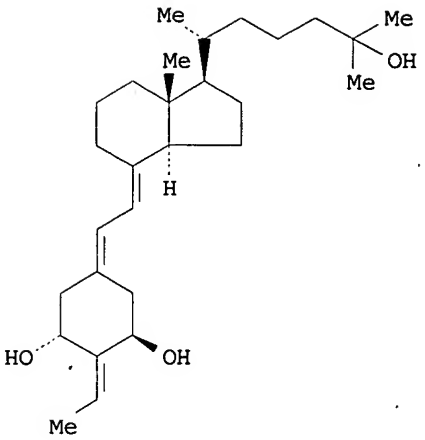


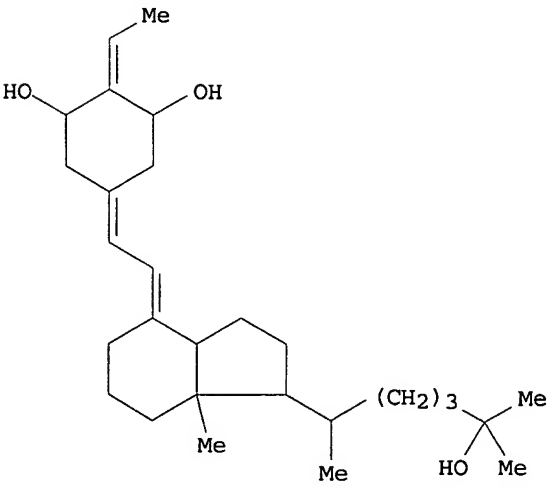
I

AB Biol. active 19-nor vitamin D analogs substituted at C-2 in the A-ring with an ethylidene or an Et group are prepared These compds. have preferential activity on mobilizing calcium from bone and either high or normal intestinal calcium transport activity which allows their in vivo administration for the treatment of metabolic bone diseases where bone loss is a major concern. These compds. are also characterized by high cell differentiation activity. Thus, I was prepared and showed high calcemic activity when tested in vivo in rats.

IT **377086-22-1P 377086-23-2P 377086-32-3P 377087-90-6P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of biol. active 2-Et and 2-ethylidene-19-norvitamin D compds.)

RN 377086-22-1 HCAPLUS

CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2E,3β)- (9CI) (CA INDEX NAME)



RN 377086-23-2 HCAPLUS

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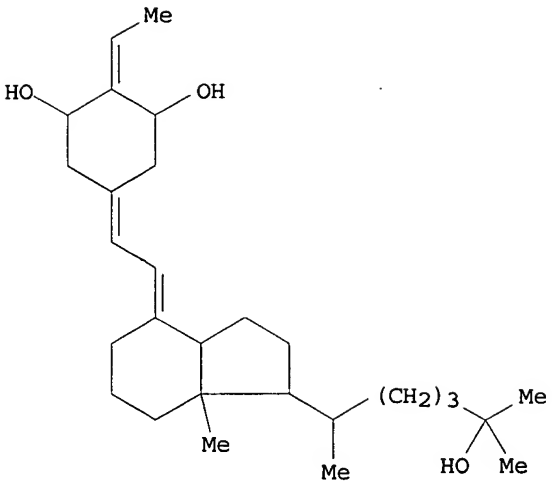
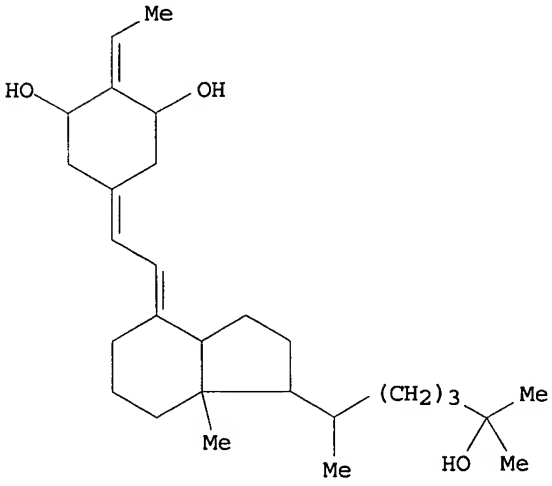
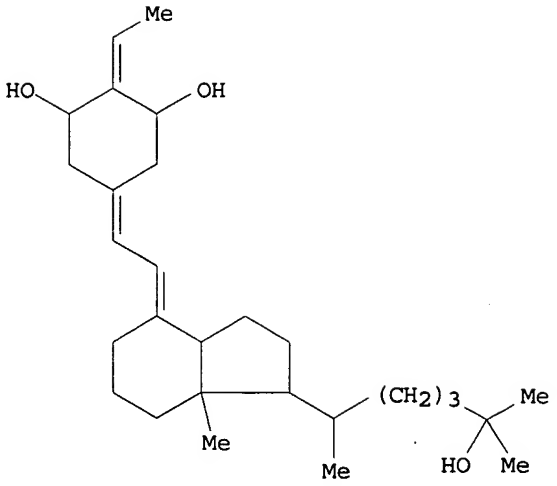


RN 377086-32-3 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2Z,3β,20S)- (9CI) (CA INDEX NAME)

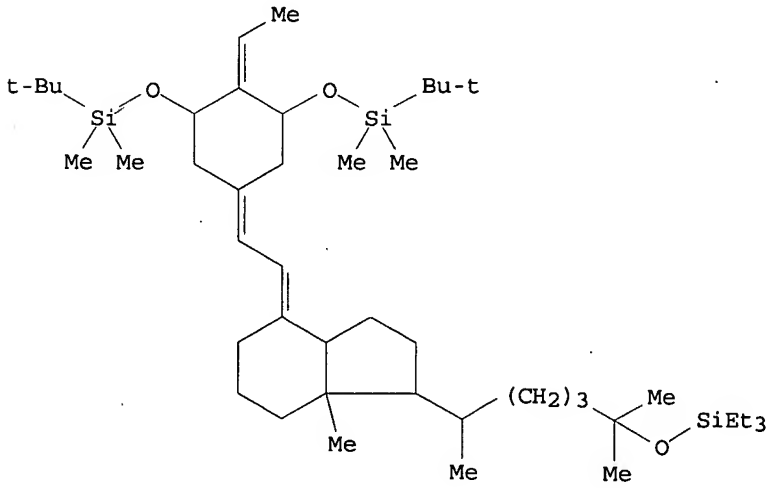


RN 377087-90-6 HCAPLUS
CN 19-Nor-9,10-secocholesta-5,7-diene-1,3,25-triol,2-ethylidene-, (1α,2E,3β,20S)- (9CI) (CA INDEX NAME)

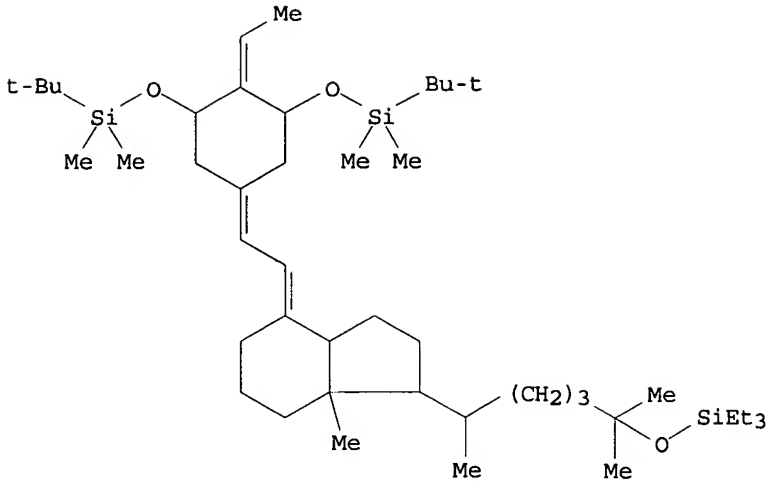


IT **377086-30-1P 377086-31-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of biol. active 2-Et and 2-ethylidene-19-norvitamin D compds.)

RN 377086-30-1 HCAPLUS
CN Silane, [[(1α,2E,3β,7E)-2-ethylidene-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



RN 377086-31-2 HCAPLUS
CN Silane, [[(1α,2Z,3β,7E)-2-ethylidene-25-[(triethylsilyl)oxy]-19-nor-9,10-secocholesta-5,7-diene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)



IC ICM C07C401-00
ICS A61K031-59
CC 32-7 (Steroids)
Section cross-reference(s): 1, 63
IT **377086-22-1P 377086-23-2P 377086-32-3P**
377087-90-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of biol. active 2-Et and 2-ethylidene-19-norvitamin D compds.)
IT 135711-62-5P 141404-07-1P 141404-08-2P 376353-72-9P
376353-73-0P 376353-74-1P 376353-75-2P 376353-76-3P
376353-77-4P 376353-78-5P 376353-79-6P 377086-26-5P
377086-27-6P 377086-28-7P 377086-29-8P **377086-30-1P**
377086-31-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of biol. active 2-Et and 2-ethylidene-19-norvitamin D compds.)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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